

10/680,076

=> d his

(FILE 'HOME' ENTERED AT 11:15:44 ON 26 SEP 2006)

FILE 'REGISTRY' ENTERED AT 11:16:05 ON 26 SEP 2006
L1 STRUCTURE UPLOADED
L2 0 S L1

FILE 'CAPLUS' ENTERED AT 11:16:51 ON 26 SEP 2006
L3 1 S US20040220164/PN
SELECT RN L3 1-

FILE 'REGISTRY' ENTERED AT 11:17:19 ON 26 SEP 2006
L4 41 S E1-41
L5 30 S L4 AND 12/SZ
L6 19728 S 12/SZ
L7 15 S L1 SUB=L6 SAM
L8 221 S L1 SUB=L6 FUL
L9 211 S L8 AND CAPLUS/LC
L10 10 S L8 NOT L9

FILE 'CAPLUS' ENTERED AT 11:20:21 ON 26 SEP 2006
L11 106 S L8
L12 ANALYZE L11 1- RN HIT : 211 TERMS

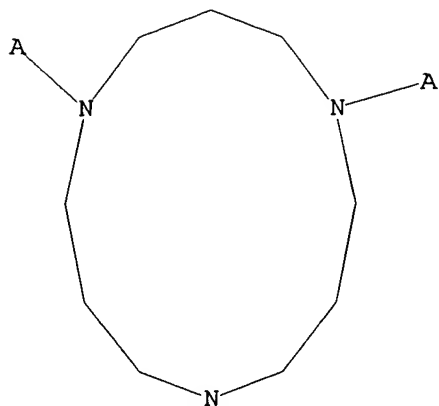
FILE 'REGISTRY' ENTERED AT 11:20:45 ON 26 SEP 2006
L13 100 S 133256?/RN
L14 1088 S 35980?/RN
L15 100 S 182316?/RN
L16 100 S 106415?/RN
L17 100 S 164913?/RN
L18 100 S 182316?/RN
L19 100 S 122114?/RN
L20 100 S 174192?/RN
L21 2 S L8 AND L13
L22 1 S L8 AND L14
L23 16 S L8 AND L15
L24 1 S L8 AND L16
L25 3 S L8 AND L17
L26 16 S L8 AND L18
L27 1 S L8 AND L19
L28 6 S L8 AND L20
L29 217 S L8 NOT (L21 OR L24 OR L27)

FILE 'CAPLUS' ENTERED AT 11:26:50 ON 26 SEP 2006
L30 83 S L29

=> d l1

L1 HAS NO ANSWERS
L1 STR

10/680,076



Structure attributes must be viewed using STN Express query preparation.

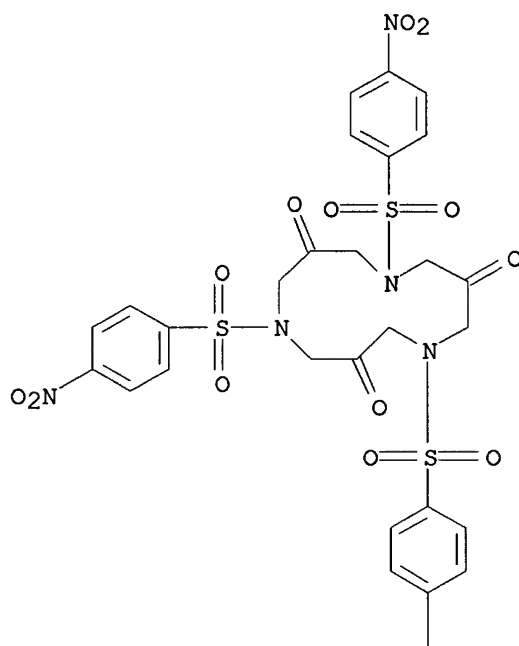
=> d 110 1-10

YOU HAVE REQUESTED DATA FROM FILE 'REGISTRY' - CONTINUE? (Y)/N:y

10/680,076

L10 ANSWER 1 OF 10 REGISTRY COPYRIGHT 2006 ACS on STN
RN 907969-73-7 REGISTRY
ED Entered STN: 20 Sep 2006
CN INDEX NAME NOT YET ASSIGNED
MF C27 H24 N6 O15 S3
SR Other Sources
Database: NCI 3D (National Cancer Institute)

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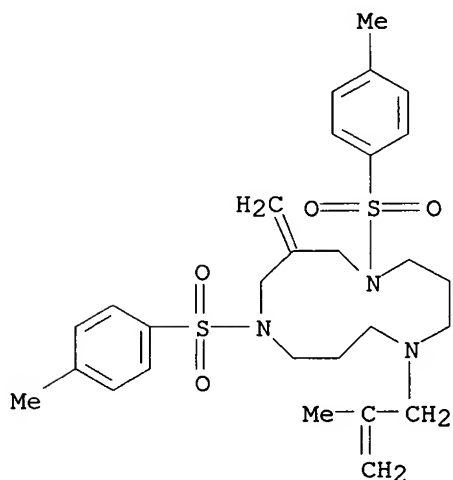
PAGE 2-A



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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L10 ANSWER 2 OF 10 REGISTRY COPYRIGHT 2006 ACS on STN
RN 907960-90-1 REGISTRY
ED Entered STN: 20 Sep 2006
CN INDEX NAME NOT YET ASSIGNED
MF C28 H39 N3 O4 S2
SR Other Sources
Database: NCI 3D (National Cancer Institute)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

10/680,076

L10 ANSWER 3 OF 10 REGISTRY COPYRIGHT 2006 ACS on STN

RN 854588-70-8 REGISTRY

ED Entered STN: 12 Jul 2005

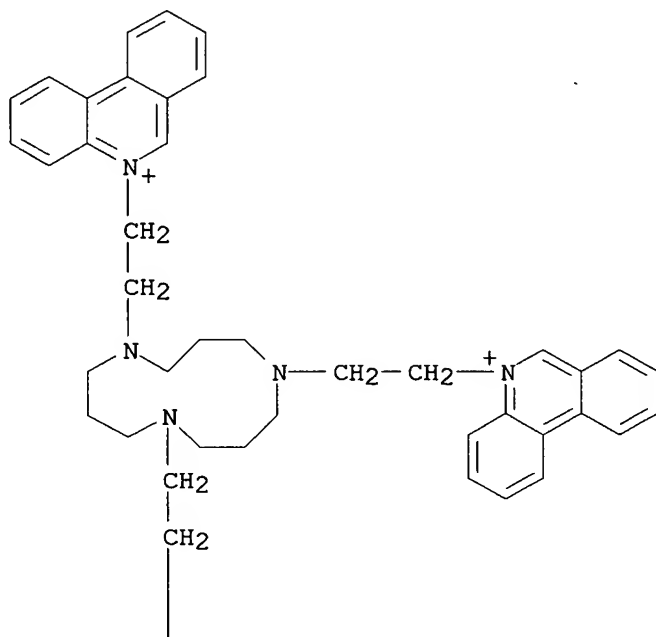
CN Phenanthridinium, 5,5',5'''-(1,5,9-triazacyclododecane-1,5,9-triyltri-2,1-ethanediyl)tris- (9CI) (CA INDEX NAME)

MF C54 H57 N6

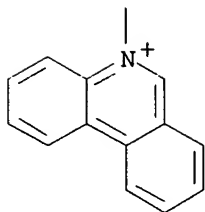
CI COM

SR CA

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PAGE 2-A



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L10 ANSWER 4 OF 10 REGISTRY COPYRIGHT 2006 ACS on STN

RN 854588-68-4 REGISTRY

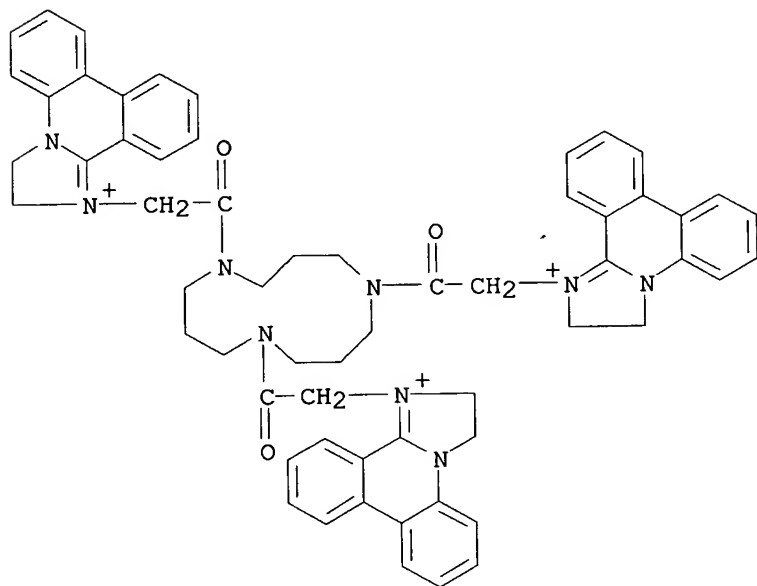
ED Entered STN: 12 Jul 2005

CN Imidazo[1,2-f]phenanthridinium, 1,1',1''-[1,5,9-triazacyclododecane-1,5,9-triyltris(2-oxo-2,1-ethanediyl)]tris[2,3-dihydro- (9CI) (CA INDEX NAME)

MF C60 H60 N9 O3

CI COM

SR CA



10/680,076

L10 ANSWER 5 OF 10 REGISTRY COPYRIGHT 2006 ACS on STN

RN 791560-02-6 REGISTRY

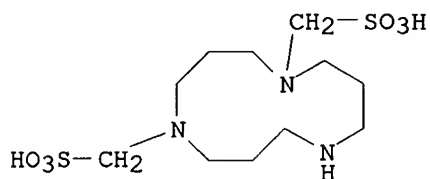
ED Entered STN: 02 Dec 2004

CN 1,5,9-Triazacyclododecane-1,5-dimethanesulfonic acid (9CI) (CA INDEX NAME)

MF C11 H25 N3 O6 S2

CI COM

SR CA



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L10 ANSWER 6 OF 10 REGISTRY COPYRIGHT 2006 ACS on STN

RN 752178-62-4 REGISTRY

ED Entered STN: 26 Sep 2004

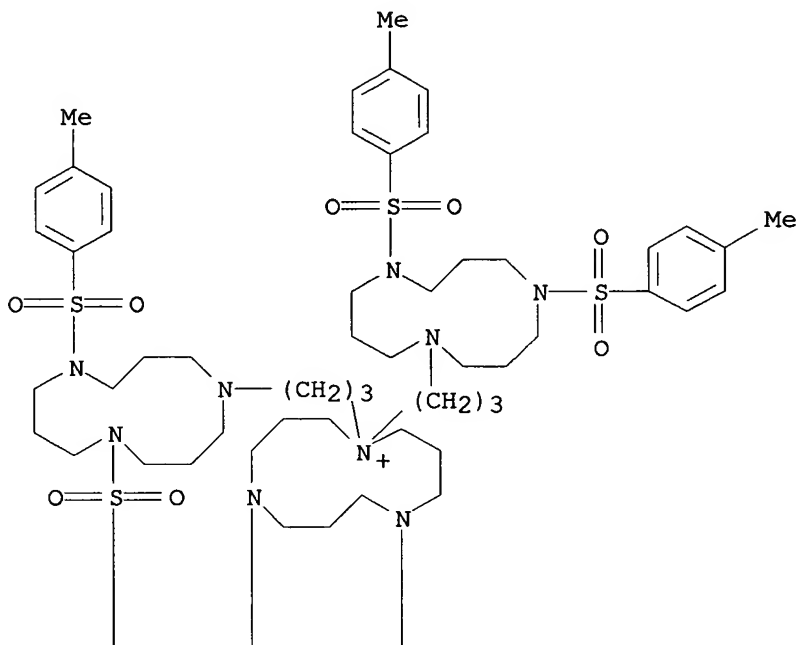
CN 5,9-Diaza-1-azonia-cyclododecane, 1,1-bis[3-[5,9-bis[(4-methylphenyl)sulfonyl]-1,5,9-triazacyclododec-1-yl]propyl]-5,9-bis[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)

MF C75 H108 N9 O12 S6

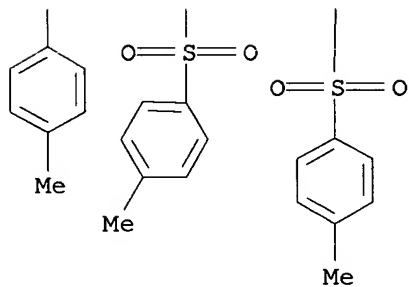
CI COM

SR CA

PAGE 1-A



PAGE 2-A



L10 ANSWER 8 OF 10 REGISTRY COPYRIGHT 2006 ACS on STN

RN 745771-41-9 REGISTRY

ED Entered STN: 16 Sep 2004

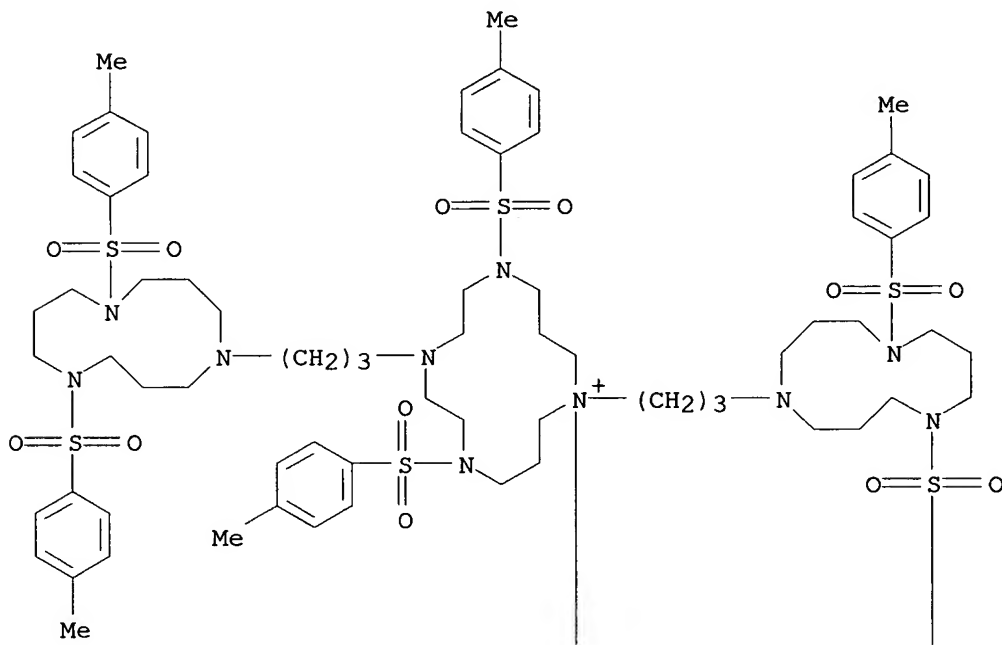
CN 1,4,7-Triaza-11-azonia-11-azacyclotetradecane, 4,11,11-tris[3-[5,9-bis[(4-methylphenyl)sulfonyl]-1,5,9-triazacyclododec-1-yl]propyl]-1,7-bis[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)

MF C102 H148 N13 O16 S8

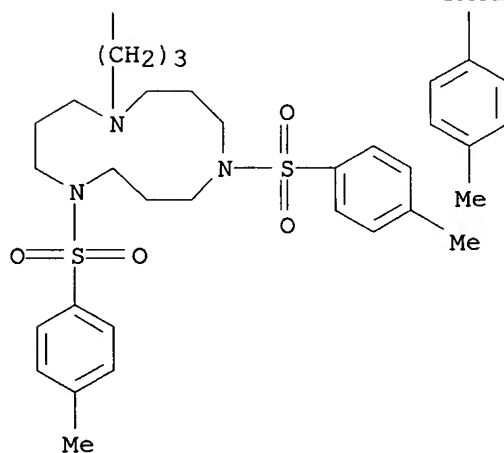
CI COM

SR CA

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PAGE 2-A



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L10 ANSWER 9 OF 10 REGISTRY COPYRIGHT 2006 ACS on STN

RN 745760-17-2 REGISTRY

ED Entered STN: 16 Sep 2004

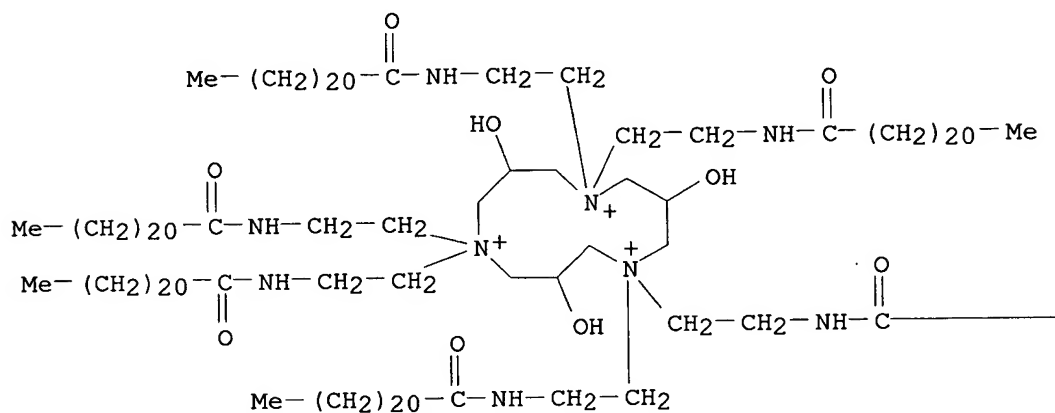
CN 1,5,9-Triazoniacyclododecane, 3,7,11-trihydroxy-1,1,5,5,9,9-hexakis[2-[(1-oxodocosyl)amino]ethyl]- (9CI) (CA INDEX NAME)

MF C153 H306 N9 O9

CI COM

SR CA

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PAGE 1-B

— (CH₂)₂₀—Me

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L10 ANSWER 10 OF 10 REGISTRY COPYRIGHT 2006 ACS on STN

RN 132434-01-6 REGISTRY

ED Entered STN: 01 Mar 1991

CN Benzoic acid, 4,4'-(1,5,9-triazacyclododecane-1,5-diylldicarbonyl)bis-
(9CI) (CA INDEX NAME)

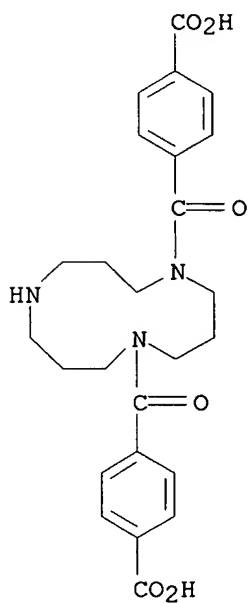
OTHER CA INDEX NAMES:

CN 1,5,9-Triazacyclododecane, benzoic acid deriv.

MF C25 H29 N3 O6

CI COM

SR CA



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

~~180~~ ANSWER 1 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2006:357496 CAPLUS

Correction of: 2005:481368

DOCUMENT NUMBER: 145:123918

Correction of: 142:481541

TITLE: Cyanogen halides, cyanates and their sulfur, selenium, and tellurium analogues, sulfinyl and sulfonyl cyanides, cyanamides, and phosphalkynes

AUTHOR(S): Wu, Y.-Q.

CORPORATE SOURCE: Dept. of Research, Guilford Pharmaceutical, Inc., Baltimore, MD, 21224, USA

SOURCE: Science of Synthesis (2005), 18, 17-63

CODEN: SSCYJ9

PUBLISHER: Georg Thieme Verlag

DOCUMENT TYPE: Journal; General Review

LANGUAGE: English

AB A review of the preparation of cyanogen halides and cyanates as well as their application to organic synthesis. Sulfur, selenium, and tellurium analogs, sulfinyl and sulfonyl cyanides, cyanamides, and phosphalkynes are included.

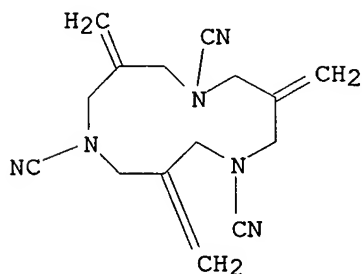
IT 219839-49-3P

RL: SPN (Synthetic preparation); PREP (Preparation)

(review preparation and application of cyanogen halides and cyanates as well as numerous derivs. thereof)

RN 219839-49-3 CAPLUS

CN 1,5,9-Triazacyclododecane-1,5,9-tricarbonitrile, 3,7,11-tris(methylene)-
(9CI) (CA INDEX NAME)



~~130~~ ANSWER 2 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2006:240977 CAPLUS

DOCUMENT NUMBER: 144:246374

TITLE: Inhibitors of HIV infection via the cellular CD4 receptor

AUTHOR(S): Vermeire, Kurt; Schols, Dominique; Bell, Thomas W.

CORPORATE SOURCE: Rega Institute for Medical Research, Katholieke Universiteit Leuven, Louvain, B-3000, Belg.

SOURCE: Current Medicinal Chemistry (2006), 13(7), 731-743
CODEN: CMCHE7; ISSN: 0929-8673

PUBLISHER: Bentham Science Publishers Ltd.

DOCUMENT TYPE: Journal; General Review

LANGUAGE: English

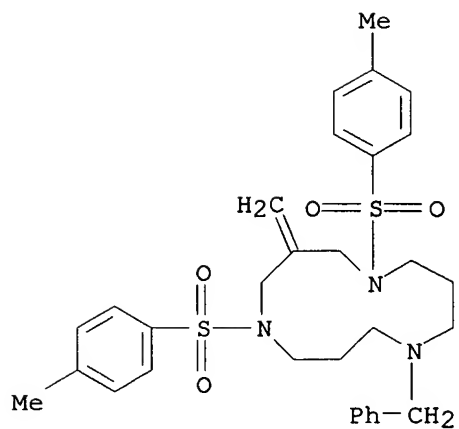
AB A review. Recent advances in the understanding of cellular and mol. mechanisms of viral penetration of the target cell have provided the basis for novel chemotherapy and prophylaxis of HIV-1 infections. This knowledge has been successfully applied to the development of inhibitors that target discrete steps of the entry process. Interesting approaches for the prevention of HIV-1 entry include the use of small-mol. inhibitors, natural ligands, and(or) monoclonal antibodies that interfere with gp120/CD4 interaction. Other compds. acting by novel mechanisms have recently been identified as anti-HIV agents and seem worthy of further preclin. development. Of particular interest in this regard are cyclotriazadisulfonamide (CADA) compds., which down-modulate the cellular receptor, CD4. A series of analogs of 9-benzyl-3-methylene-1,5-di-p-toluenesulfonyl-1,5,9-triazacyclododecane (CADA) has been synthesized and tested for CD4 down-modulation and anti-HIV activity. Some derivs. proved to be highly effective in decreasing cellular CD4 and in acting as HIV entry inhibitors. Three-dimensional quant. structure-activity relationship (3D-QSAR) studies correlating mol. features with potency have been used to produce a computational model. This model can be used to design more potent CD4 down-modulating drugs for HIV therapy and prophylaxis. This review summarizes the results of recent studies relating to inhibitors of HIV infection via CD4 and discusses the therapeutic potential of targeting this cellular receptor. Special attention is given to the authors' own work on small-mol. HIV entry inhibitors endowed with CD4 down-modulating properties.

IT 182316-44-5, CADA

RL: DMA (Drug mechanism of action); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(inhibitors of HIV infection via cellular CD4 receptor)

RN 182316-44-5 CAPLUS

CN 1,5,9-Triazacyclododecane, 3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]-9-(phenylmethyl)- (9CI) (CA INDEX NAME)



REFERENCE COUNT:

102

THERE ARE 102 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE REFORMAT

~~L76~~ ANSWER 3 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2006:94623 CAPLUS

DOCUMENT NUMBER: 144:350657

TITLE: Synthesis and Structure-Activity Relationship Studies of CD4 Down-Modulating Cyclotriazadisulfonamide (CADA) Analogues

AUTHOR(S): Bell, Thomas W.; Anugu, Sreenivasa; Bailey, Patrick; Catalano, Vincent J.; Dey, Kaka; Drew, Michael G. B.; Duffy, Noah H.; Jin, Qi; Samala, Meinrado F.; Sodoma, Andrej; Welch, William H.; Schols, Dominique; Vermeire, Kurt

CORPORATE SOURCE: Departments of Chemistry and Biochemistry, University of Nevada, Reno, NV, 89557, USA

SOURCE: Journal of Medicinal Chemistry (2006), 49(4), 1291-1312

CODEN: JMCMAR; ISSN: 0022-2623

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 144:350657

AB HIV attachment via the CD4 receptor is an important target for developing novel approaches to HIV chemotherapy. Cyclotriazadisulfonamide (CADA) inhibits HIV at sub-micromolar levels by specifically down-modulating cell-surface and intracellular CD4. An effective five-step synthesis of CADA in 30% overall yield is reported. This synthesis has also been modified to produce more than 50 analogs. Many tail-group analogs have been made by removing the benzyl tail of CADA and replacing it with various alkyl, acyl, alkoxycarbonyl and aminocarbonyl substituents. A series of sidearm analogs, including two unsym. compds., have also been prepared by modifying the CADA synthesis, replacing the toluenesulfonyl sidearms with other sulfonyl groups. Testing 30 of these compds. in MT-4 cells shows a wide range of CD4 down-modulation potency, which correlates with ability to inhibit HIV-1. Three-dimensional quant. structure-activity relationship (3D-QSAR) models were constructed using comparative mol. field anal. (CoMFA) and comparative mol. similarity indexes anal. (CoMSIA) approaches. The X-ray crystal structures of four compds., including CADA, show the same major conformation of the central 12-membered ring. The solid-state structure of CADA was energy minimized and used to generate the remaining 29 structures, which were similarly minimized and aligned to produce the 3D-QSAR models. Both models indicate that steric bulk of the tail group, and, to a lesser extent, the sidearms mainly determine CD4 down-modulation potency in this series of compds.

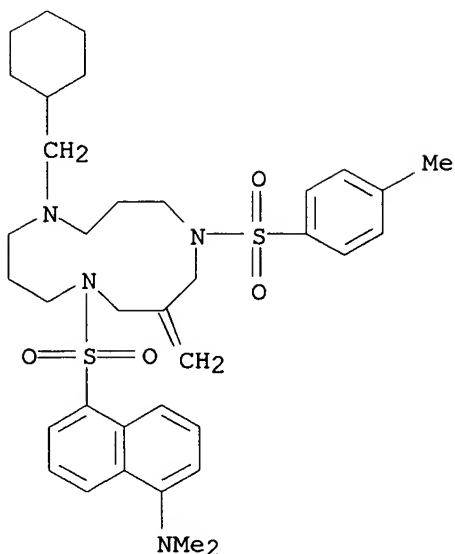
IT 471866-80-5P 881693-80-7P

RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)

(preparation and structure-activity relationship study of CD4 down-modulating cyclotriazadisulfonamide (CADA) analogs)

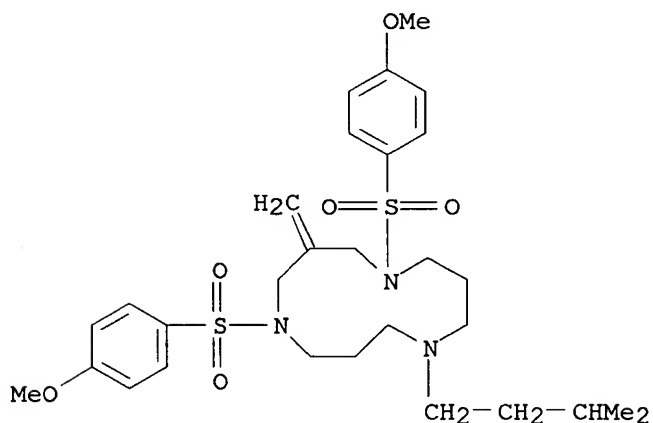
RN 471866-80-5 CAPLUS

CN 1,5,9-Triazacyclododecane, 9-(cyclohexylmethyl)-1-[[5-(dimethylamino)-1-naphthalenyl]sulfonyl]-3-methylene-5-[(4-methylphenyl)sulfonyl]- (9CI)
(CA INDEX NAME)



RN 881693-80-7 CAPLUS

CN 1,5,9-Triazacyclododecane, 1,5-bis[(4-methoxyphenyl)sulfonyl]-9-(3-methylbutyl)-3-methylene- (9CI) (CA INDEX NAME)



IT 182316-44-5DP, CADA, analogs 471866-79-2P

881693-78-3P 881693-79-4P 881693-81-8P

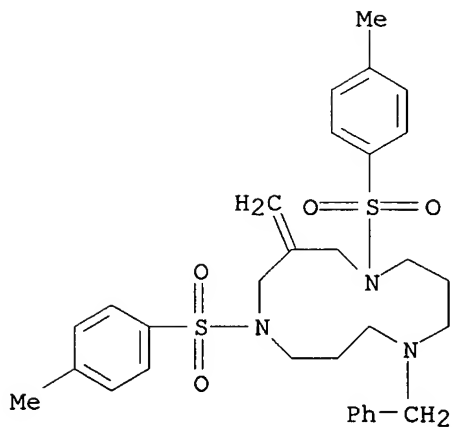
881693-82-9P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(preparation and structure-activity relationship study of CD4 down-modulating cyclotriazadisulfonamide (CADA) analogs)

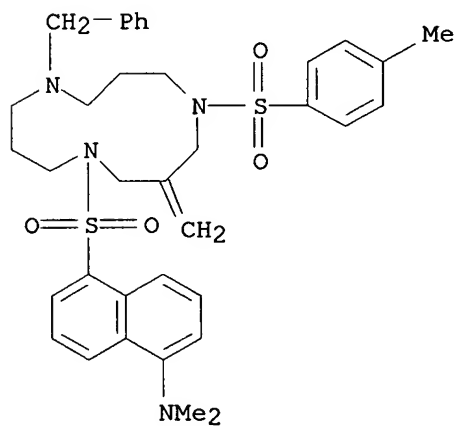
RN 182316-44-5 CAPLUS

CN 1,5,9-Triazacyclododecane, 3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]-9-(phenylmethyl)- (9CI) (CA INDEX NAME)



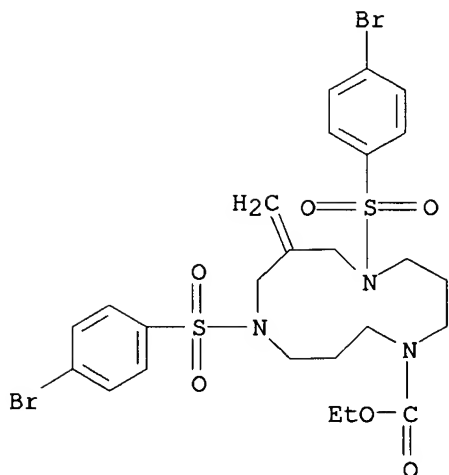
RN 471866-79-2 CAPLUS

CN 1,5,9-Triazacyclododecane, 1-[[5-(dimethylamino)-1-naphthalenyl]sulfonyl]-3-methylene-5-[(4-methylphenyl)sulfonyl]-9-(phenylmethyl)- (9CI) (CA INDEX NAME)



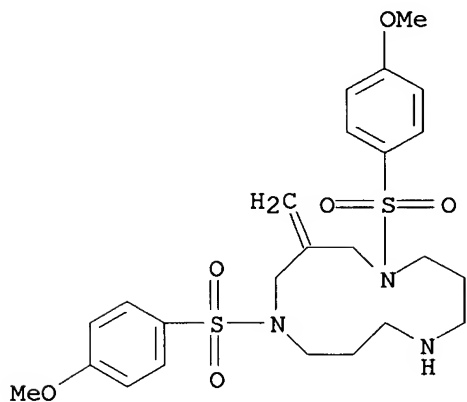
RN 881693-78-3 CAPLUS

CN 1,5,9-Triazacyclododecane-1-carboxylic acid, 5,9-bis[(4-bromophenyl)sulfonyl]-7-methylene-, ethyl ester (9CI) (CA INDEX NAME)



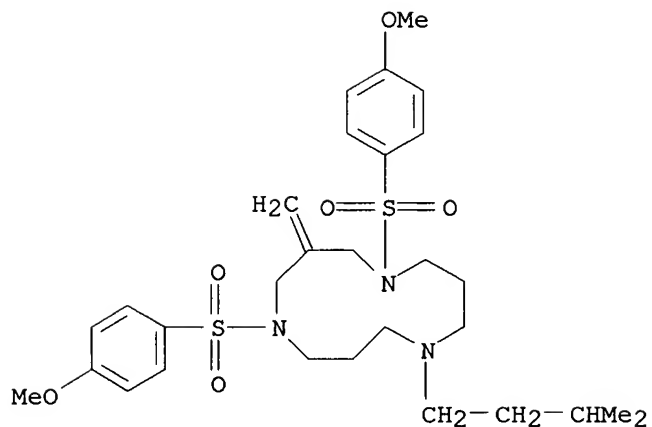
RN 881693-79-4 CAPLUS

CN 1,5,9-Triazacyclododecane, 1,5-bis[(4-methoxyphenyl)sulfonyl]-3-methylene- (9CI) (CA INDEX NAME)



RN 881693-81-8 CAPLUS

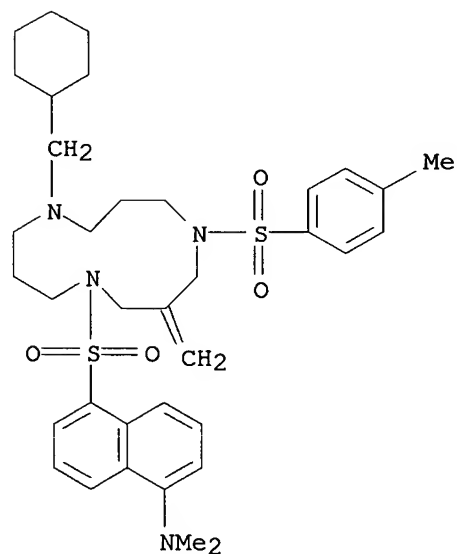
CN 1,5,9-Triazacyclododecane, 1,5-bis[(4-methoxyphenyl)sulfonyl]-9-(3-methylbutyl)-3-methylene-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 881693-82-9 CAPLUS

CN 1,5,9-Triazacyclododecane, 9-(cyclohexylmethyl)-1-[[5-(dimethylamino)-1-naphthalenyl]sulfonyl]-3-methylene-5-[(4-methylphenyl)sulfonyl]-, dihydrochloride (9CI) (CA INDEX NAME)



● 2 HCl

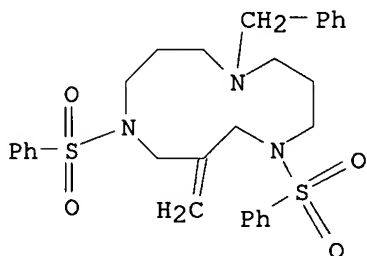
IT 182316-34-3P 182316-50-3P 392287-04-6P
 471866-90-7P 471866-91-8P 471866-93-0P
 471866-97-4P 471867-00-2P 471867-03-5P
 471867-04-6P 471867-06-8P 881693-37-4P
 881693-38-5P 881693-39-6P 881693-54-5P
 881693-55-6P 881693-56-7P 881693-57-8P
 881693-58-9P 881693-59-0P 881693-62-5P
 881693-72-7P 881693-74-9P 881693-76-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

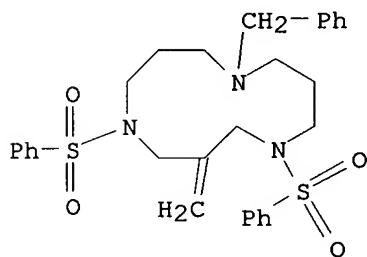
(Reactant or reagent)

(preparation and structure-activity relationship study of CD4
down-modulating cyclotriazadisulfonamide (CADA) analogs)

RN 182316-34-3 CAPLUS

CN 1,5,9-Triazacyclododecane, 3-methylene-9-(phenylmethyl)-1,5-
bis(phenylsulfonyl)- (9CI) (CA INDEX NAME)

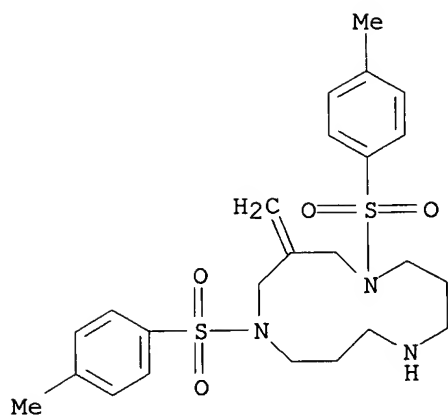
RN 182316-50-3 CAPLUS

CN 1,5,9-Triazacyclododecane, 3-methylene-9-(phenylmethyl)-1,5-
bis(phenylsulfonyl)-, monohydrochloride (9CI) (CA INDEX NAME)

● HCl

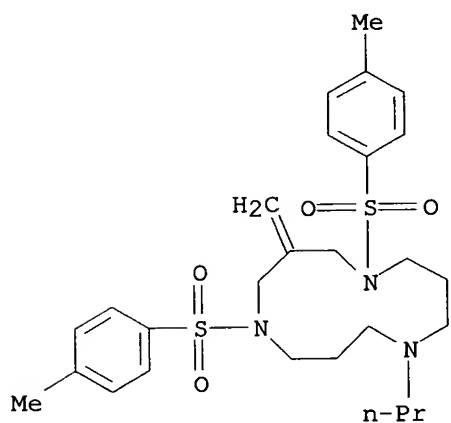
RN 392287-04-6 CAPLUS

CN 1,5,9-Triazacyclododecane, 3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]-,
monohydrochloride (9CI) (CA INDEX NAME)

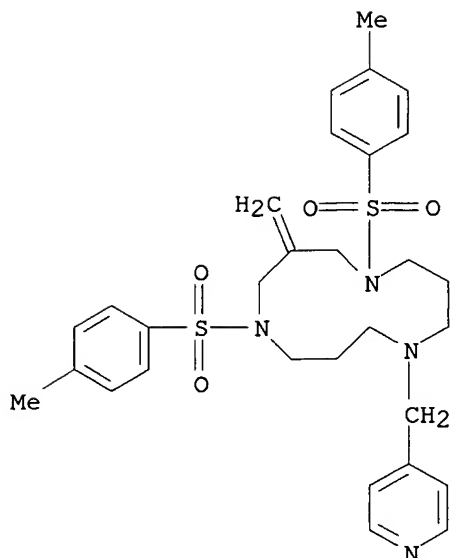


● HCl

RN 471866-90-7 CAPLUS
 CN 1,5,9-Triazacyclododecane, 3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]-9-propyl- (9CI) (CA INDEX NAME)

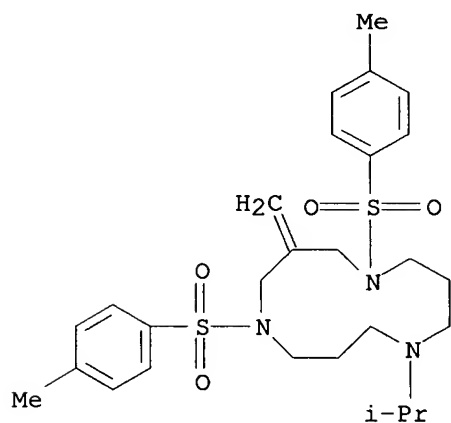


RN 471866-91-8 CAPLUS
 CN 1,5,9-Triazacyclododecane, 3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]-9-(4-pyridinylmethyl)- (9CI) (CA INDEX NAME)



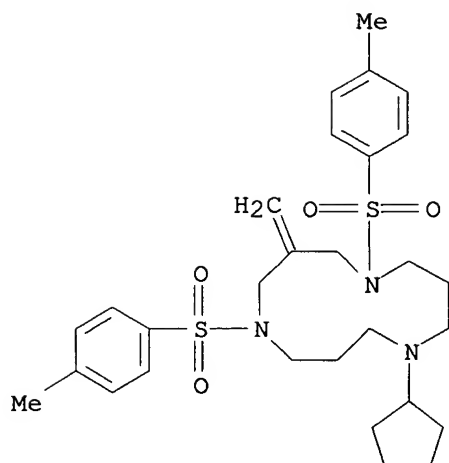
RN 471866-93-0 CAPLUS

CN 1,5,9-Triazacyclododecane, 3-methylene-9-(1-methylethyl)-1,5-bis[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)



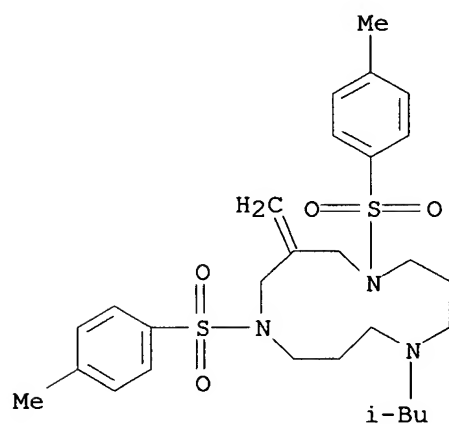
RN 471866-97-4 CAPLUS

CN 1,5,9-Triazacyclododecane, 9-cyclopentyl-3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)



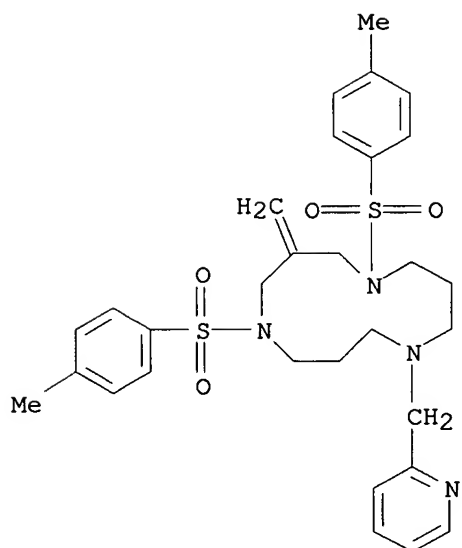
RN 471867-00-2 CAPLUS

CN 1,5,9-Triazacyclododecane, 3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]-9-(2-methylpropyl)- (9CI) (CA INDEX NAME)

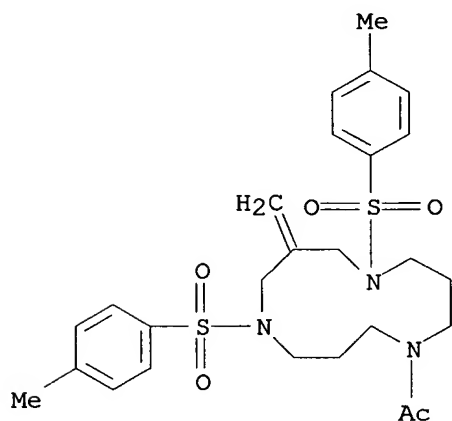


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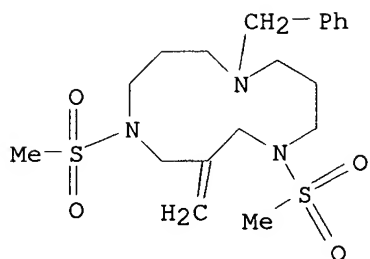
CN 1,5,9-Triazacyclododecane, 3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]-9-(2-pyridinylmethyl)- (9CI) (CA INDEX NAME)



RN 471867-04-6 CAPLUS
 CN 1,5,9-Triazacyclododecane, 9-acetyl-3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)

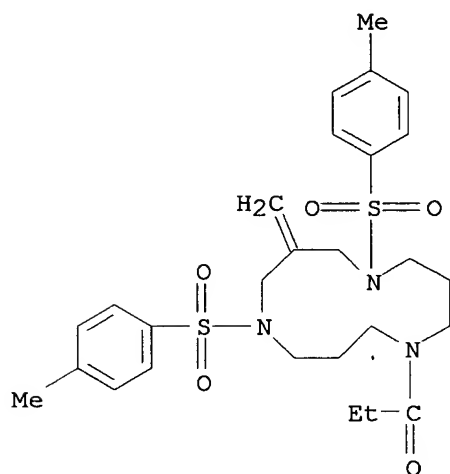


RN 471867-06-8 CAPLUS
 CN 1,5,9-Triazacyclododecane, 3-methylene-1,5-bis(methylsulfonyl)-9-(phenylmethyl)- (9CI) (CA INDEX NAME)



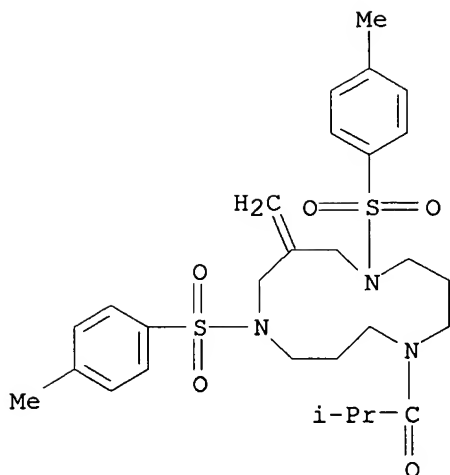
RN 881693-37-4 CAPLUS

CN 1,5,9-Triazacyclododecane, 3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]-9-(1-oxopropyl)- (9CI) (CA INDEX NAME)



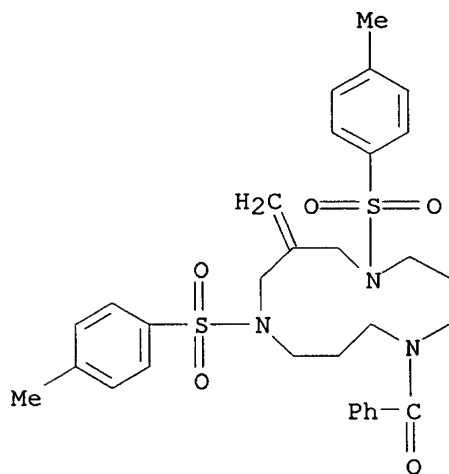
RN 881693-38-5 CAPLUS

CN 1,5,9-Triazacyclododecane, 3-methylene-9-(2-methyl-1-oxopropyl)-1,5-bis[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)



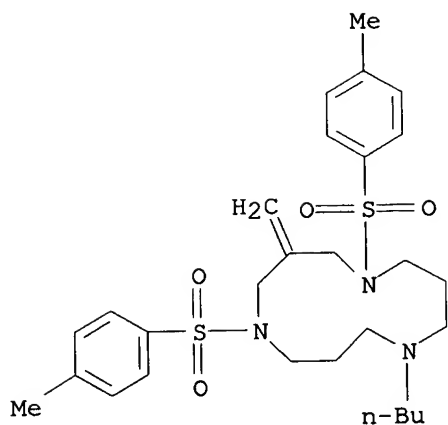
RN 881693-39-6 CAPLUS

CN 1,5,9-Triazacyclododecane, 9-benzoyl-3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)



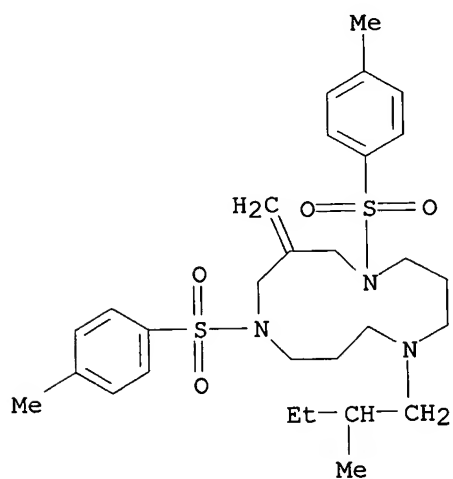
RN 881693-54-5 CAPLUS

CN 1,5,9-Triazacyclododecane, 9-butyl-3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]-, monohydrochloride (9CI) (CA INDEX NAME)



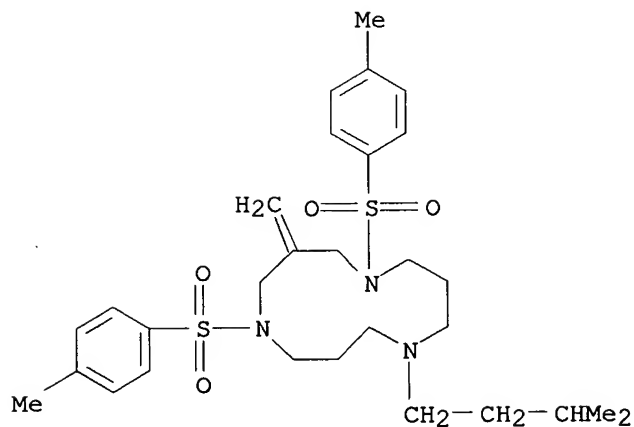
● HCl

RN 881693-55-6 CAPLUS
 CN 1,5,9-Triazacyclododecane, 9-(2-methylbutyl)-3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]-, monohydrochloride (9CI) (CA INDEX NAME)



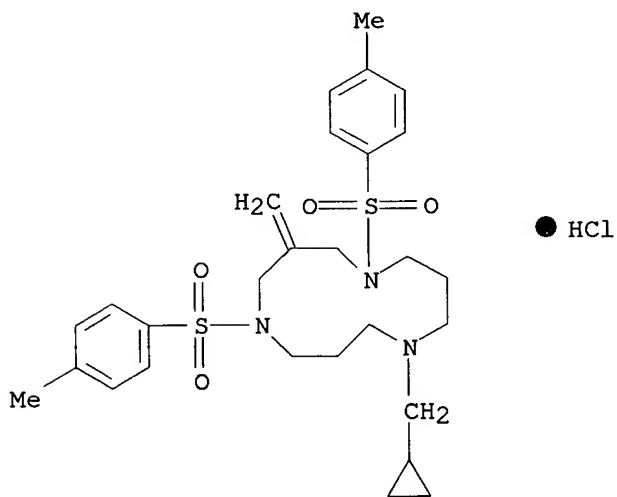
● HCl

RN 881693-56-7 CAPLUS
 CN 1,5,9-Triazacyclododecane, 9-(3-methylbutyl)-3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]-, monohydrochloride (9CI) (CA INDEX NAME)



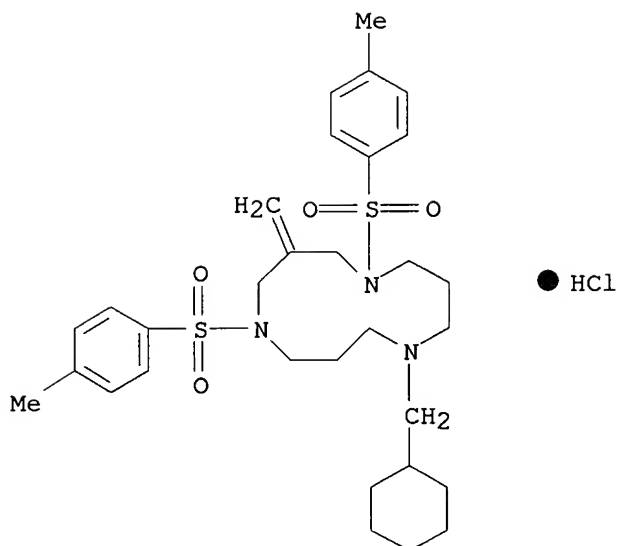
RN 881693-57-8 CAPLUS

CN 1,5,9-Triazacyclododecane, 9-(cyclopropylmethyl)-3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]-, monohydrochloride (9CI) (CA INDEX NAME)

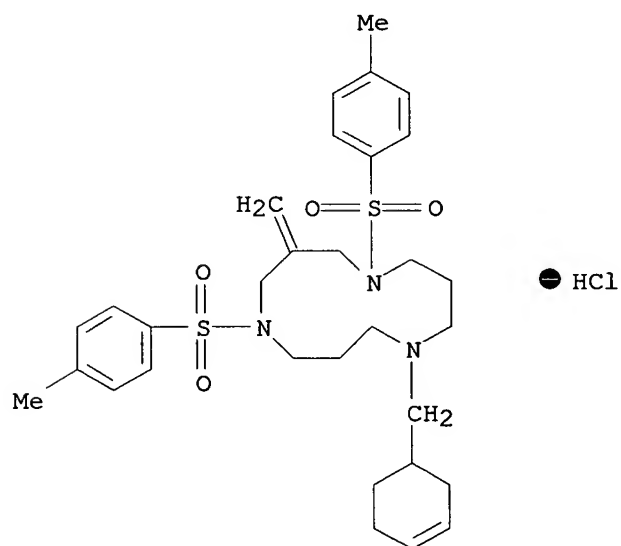


RN 881693-58-9 CAPLUS

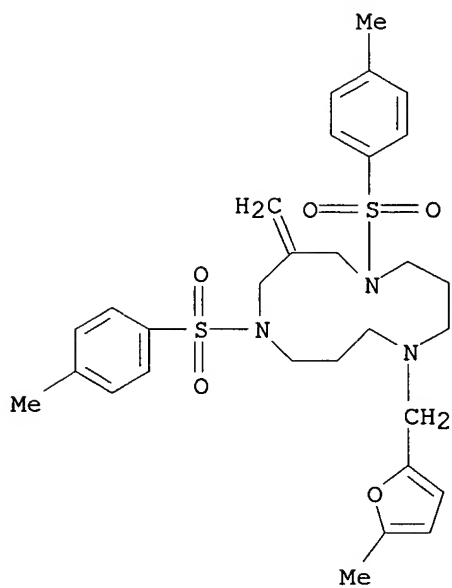
CN 1,5,9-Triazacyclododecane, 9-(cyclohexylmethyl)-3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]-, monohydrochloride (9CI) (CA INDEX NAME)



RN 881693-59-0 CAPLUS
 CN 1,5,9-Triazacyclododecane, 9-(3-cyclohexen-1-ylmethyl)-3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]-, monohydrochloride (9CI) (CA INDEX NAME)

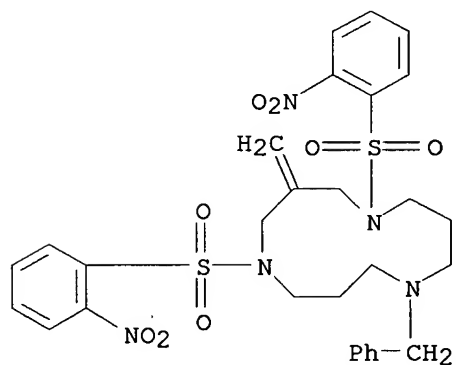


RN 881693-62-5 CAPLUS
 CN 1,5,9-Triazacyclododecane, 3-methylene-9-[(5-methyl-2-furanyl)methyl]-1,5-bis[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)



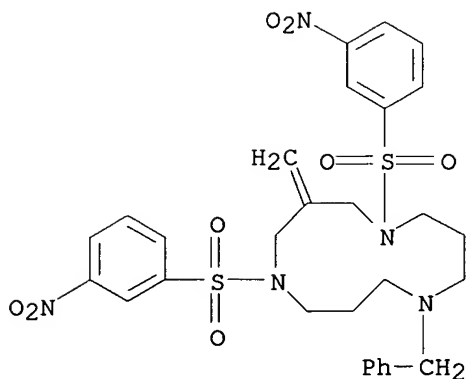
RN 881693-72-7 CAPLUS

CN 1,5,9-Triazacyclododecane, 3-methylene-1,5-bis[(2-nitrophenyl)sulfonyl]-9-(phenylmethyl)- (9CI) (CA INDEX NAME)



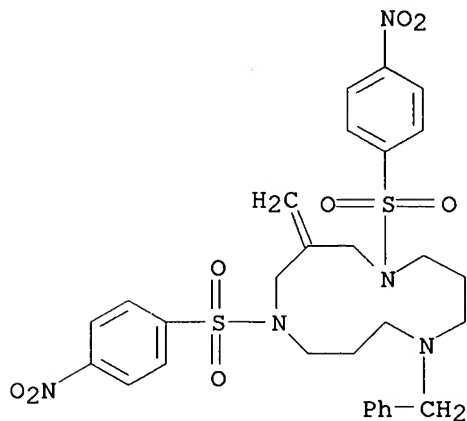
RN 881693-74-9 CAPLUS

CN 1,5,9-Triazacyclododecane, 3-methylene-1,5-bis[(3-nitrophenyl)sulfonyl]-9-(phenylmethyl)- (9CI) (CA INDEX NAME)



RN 881693-76-1 CAPLUS

CN 1,5,9-Triazacyclododecane, 3-methylene-1,5-bis[(4-nitrophenyl)sulfonyl]-9-(phenylmethyl)- (9CI) (CA INDEX NAME)



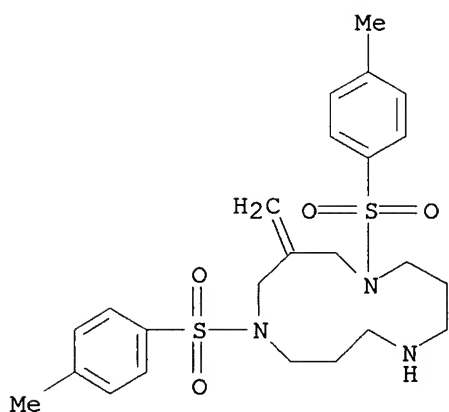
IT 182316-06-9P 182316-30-9P 392287-03-5P
 471866-86-1P 471866-87-2P 471866-89-4P
 471866-92-9P 471866-94-1P 471866-95-2P
 471866-96-3P 471866-98-5P 471867-05-7P
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 881693-28-3P 881693-29-4P 881693-30-7P
 881693-31-8P 881693-32-9P 881693-33-0P
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 881693-51-2P 881693-52-3P 881693-53-4P
 881693-60-3P 881693-61-4P 881693-63-6P
 881693-64-7P 881693-65-8P 881693-66-9P
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 881693-77-2P 881693-83-0P

RL: SPN (Synthetic preparation); PREP (Preparation)

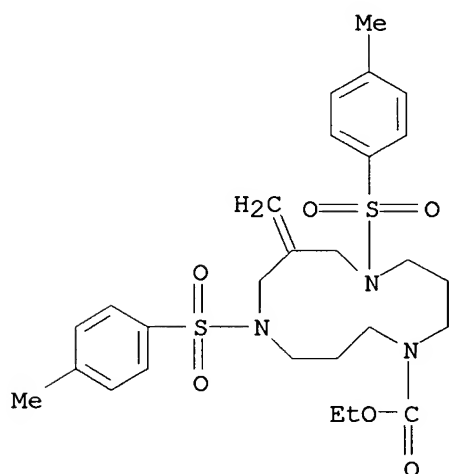
(preparation and structure-activity relationship study of CD4 down-modulating cyclotriazadisulfonamide (CADA) analogs)

RN 182316-06-9 CAPLUS

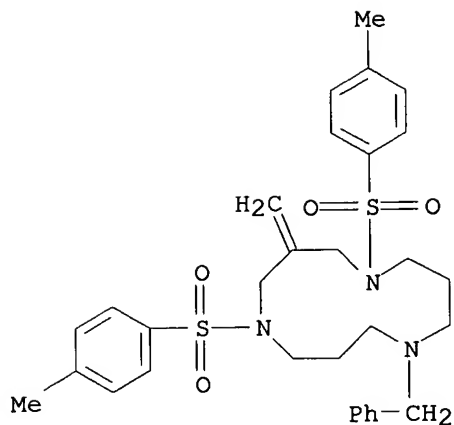
CN 1,5,9-Triazacyclododecane, 3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)



RN 182316-30-9 CAPLUS
 CN 1,5,9-Triazacyclododecane-1-carboxylic acid, 7-methylene-5,9-bis[(4-methylphenyl)sulfonyl]-, ethyl ester (9CI) (CA INDEX NAME)

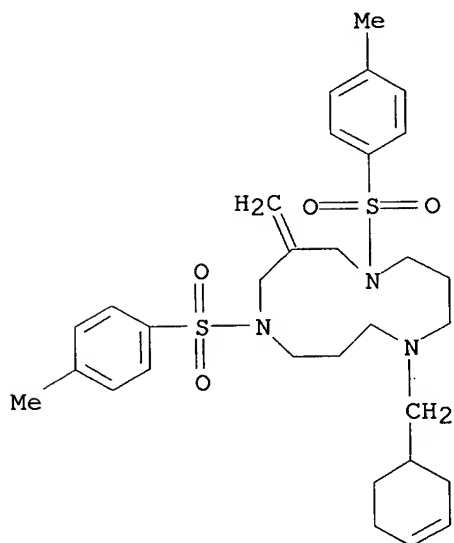


RN 392287-03-5 CAPLUS
 CN 1,5,9-Triazacyclododecane, 3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]-9-(phenylmethyl)-, monohydrochloride (9CI) (CA INDEX NAME)

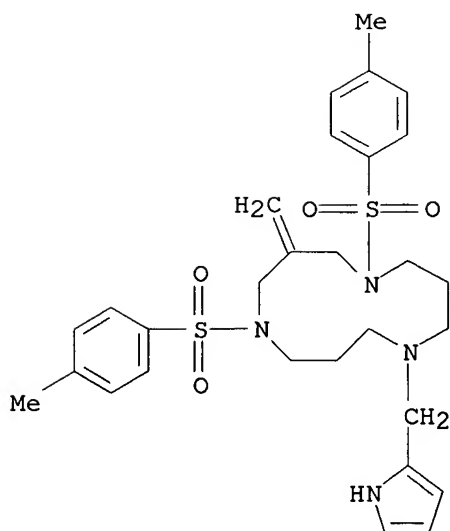


● HCl

RN 471866-86-1 CAPLUS
 CN 1,5,9-Triazacyclododecane, 9-(3-cyclohexen-1-ylmethyl)-3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)

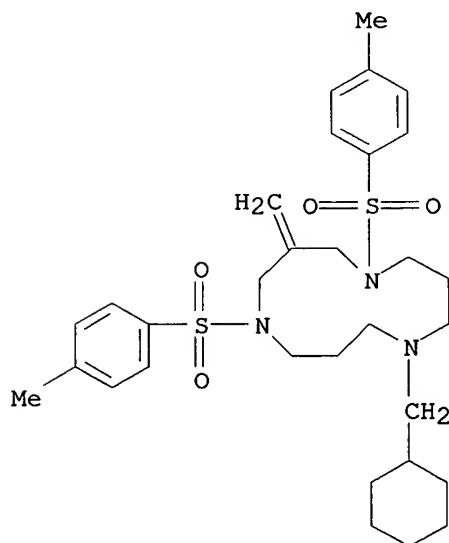


RN 471866-87-2 CAPLUS
 CN 1,5,9-Triazacyclododecane, 3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]-9-(1H-pyrrol-2-ylmethyl)- (9CI) (CA INDEX NAME)



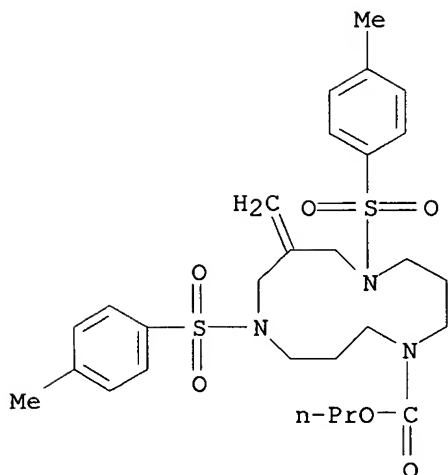
RN 471866-89-4 CAPLUS

CN 1,5,9-Triazacyclododecane, 9-(cyclohexylmethyl)-3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)



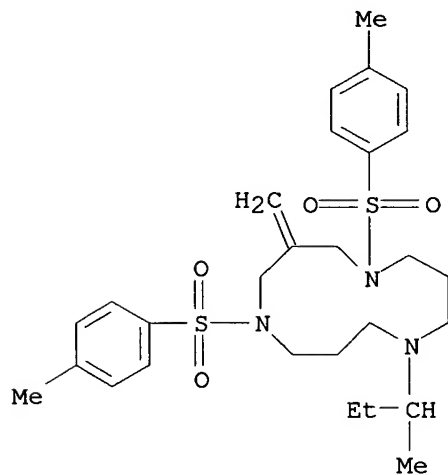
RN 471866-92-9 CAPLUS

CN 1,5,9-Triazacyclododecane-1-carboxylic acid, 7-methylene-5,9-bis[(4-methylphenyl)sulfonyl]-, propyl ester (9CI) (CA INDEX NAME)



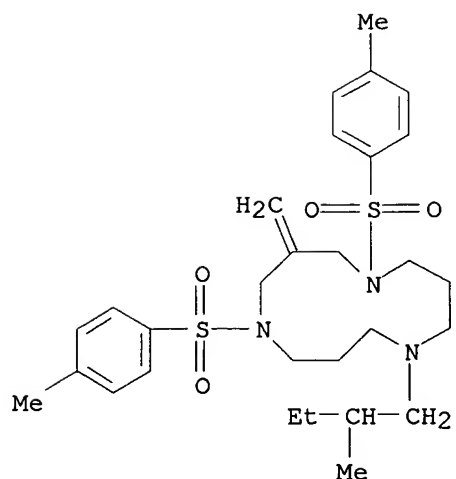
RN 471866-94-1 CAPLUS

CN 1,5,9-Triazacyclododecane, 3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]-9-(1-methylpropyl)- (9CI) (CA INDEX NAME)



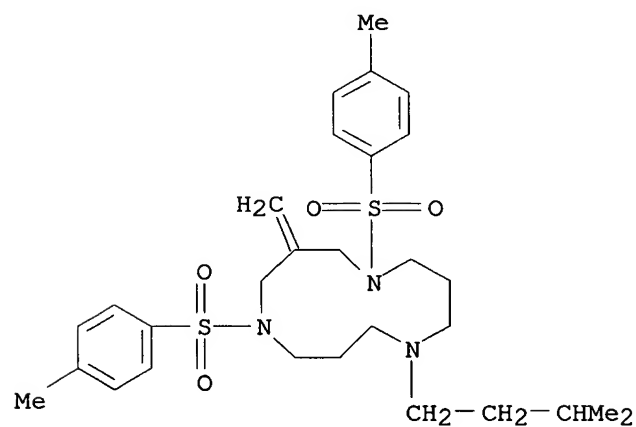
RN 471866-95-2 CAPLUS

CN 1,5,9-Triazacyclododecane, 9-(2-methylbutyl)-3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)



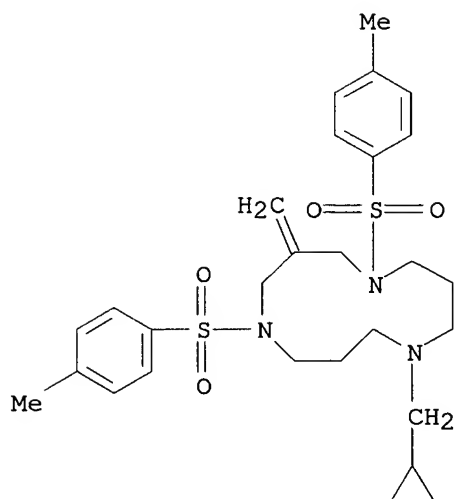
RN 471866-96-3 CAPLUS

CN 1,5,9-Triazacyclododecane, 9-(3-methylbutyl)-3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)



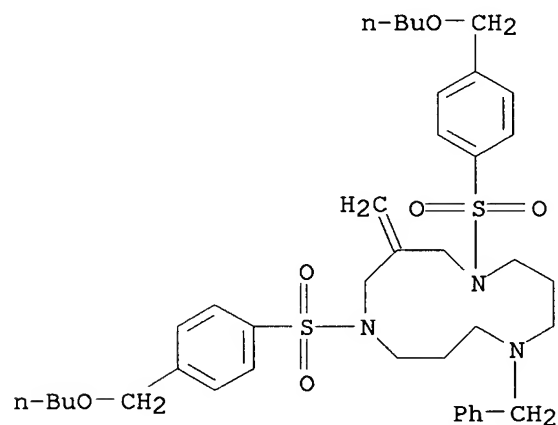
RN 471866-98-5 CAPLUS

CN 1,5,9-Triazacyclododecane, 9-(cyclopropylmethyl)-3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)



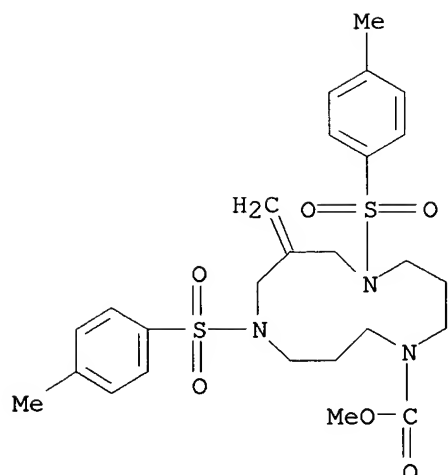
RN 471867-05-7 CAPLUS

CN 1,5,9-Triazacyclododecane, 1,5-bis[[4-(butoxymethyl)phenyl]sulfonyl]-3-methylene-9-(phenylmethyl)- (9CI) (CA INDEX NAME)



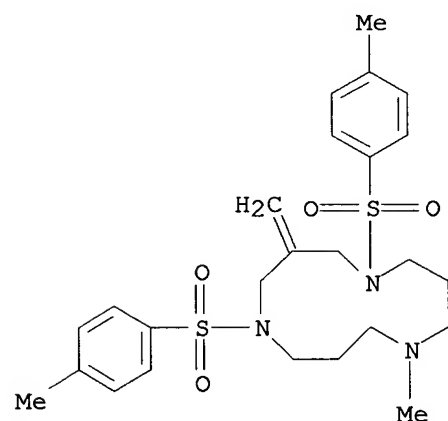
RN 881693-25-0 CAPLUS

CN 1,5,9-Triazacyclododecane-1-carboxylic acid, 7-methylene-5,9-bis[(4-methylphenyl)sulfonyl]-, methyl ester (9CI) (CA INDEX NAME)



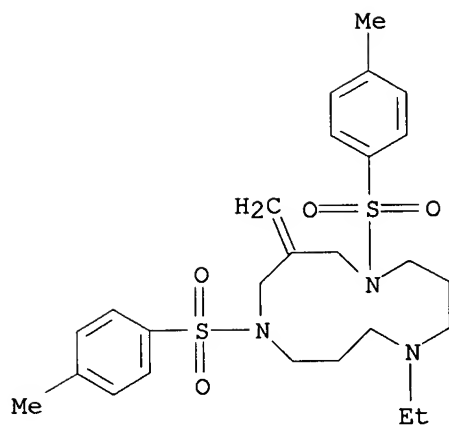
RN 881693-26-1 CAPLUS

CN 1,5,9-Triazacyclododecane, 9-methyl-3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)



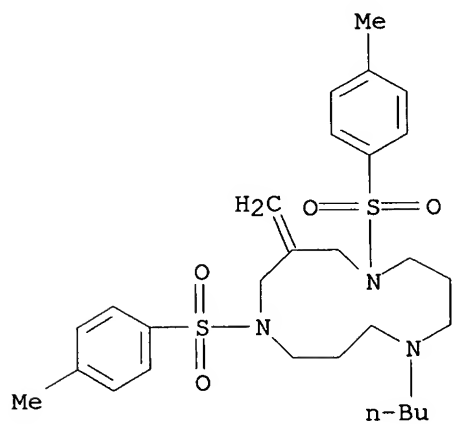
RN 881693-27-2 CAPLUS

CN 1,5,9-Triazacyclododecane, 9-ethyl-3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)



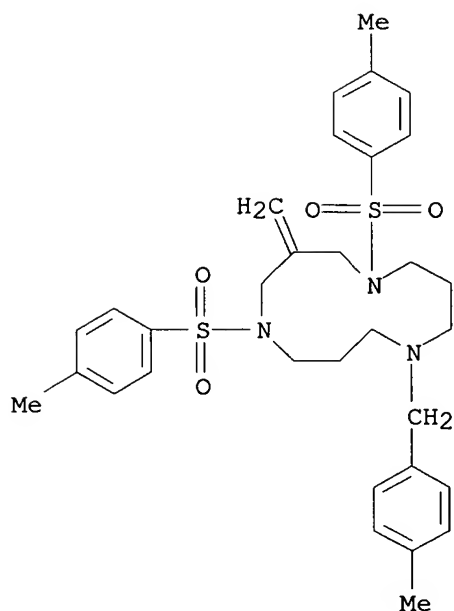
RN 881693-28-3 CAPLUS

CN 1,5,9-Triazacyclododecane, 9-butyl-3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)

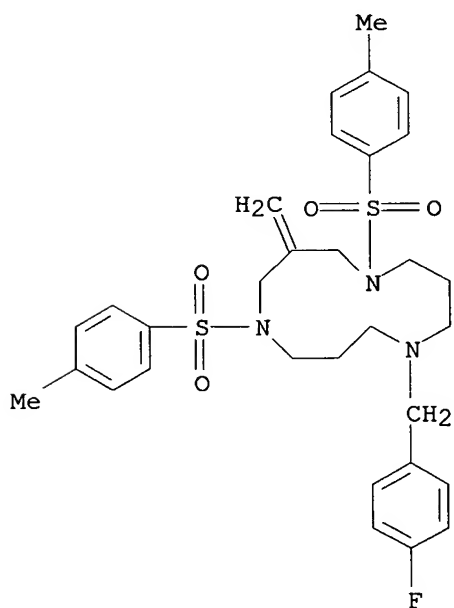


RN 881693-29-4 CAPLUS

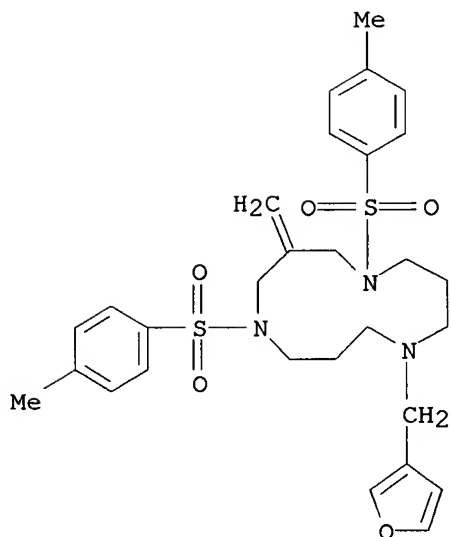
CN 1,5,9-Triazacyclododecane, 3-methylene-9-[(4-methylphenyl)methyl]-1,5-bis[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)



RN 881693-30-7 CAPLUS
 CN 1,5,9-Triazacyclododecane, 9-[(4-fluorophenyl)methyl]-3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)

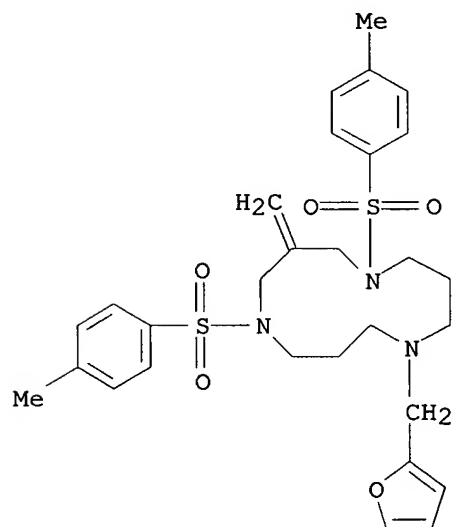


RN 881693-31-8 CAPLUS
 CN 1,5,9-Triazacyclododecane, 9-(3-furanylmethyl)-3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)



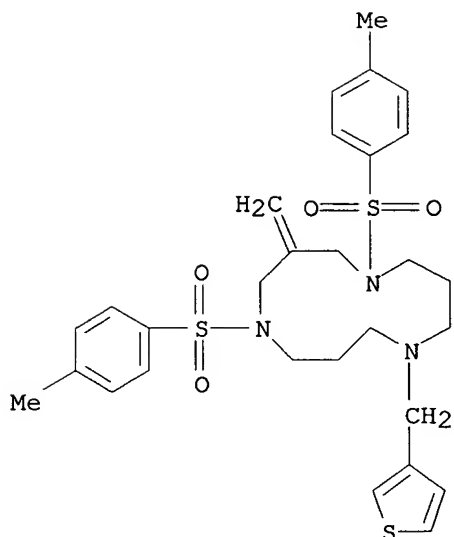
RN 881693-32-9 CAPLUS

CN 1,5,9-Triazacyclododecane, 9-(2-furanylmethyl)-3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)



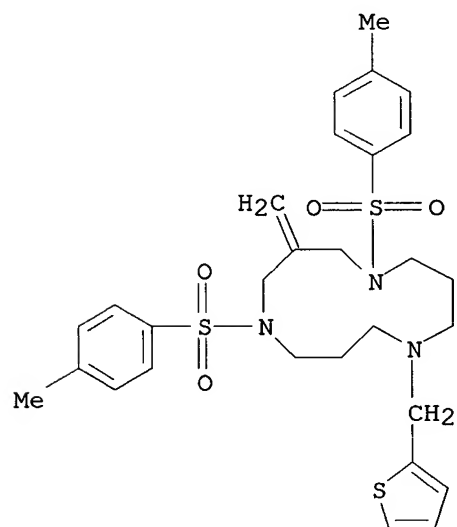
RN 881693-33-0 CAPLUS

CN 1,5,9-Triazacyclododecane, 3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]-9-(3-thienylmethyl)- (9CI) (CA INDEX NAME)



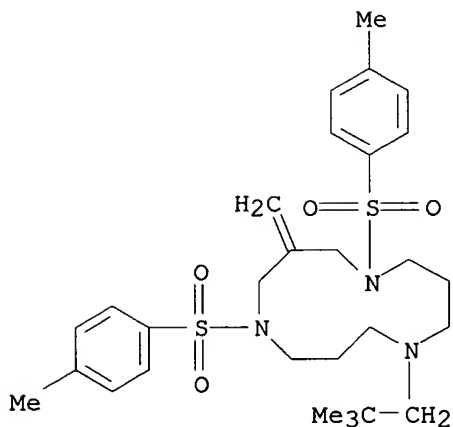
RN 881693-34-1 CAPLUS

CN 1,5,9-Triazacyclododecane, 3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]-9-(2-thienylmethyl)- (9CI) (CA INDEX NAME)



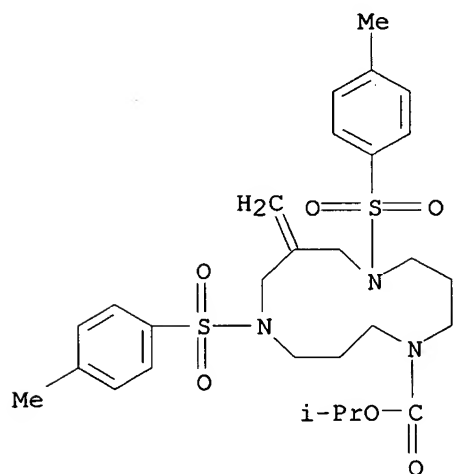
RN 881693-36-3 CAPLUS

CN 1,5,9-Triazacyclododecane, 9-(2,2-dimethylpropyl)-3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)



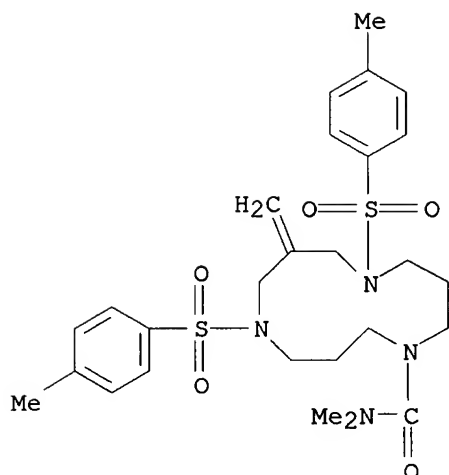
RN 881693-40-9 CAPLUS

CN 1,5,9-Triazacyclododecane-1-carboxylic acid, 7-methylene-5,9-bis[(4-methylphenyl)sulfonyl]-, 1-methylethyl ester (9CI) (CA INDEX NAME)



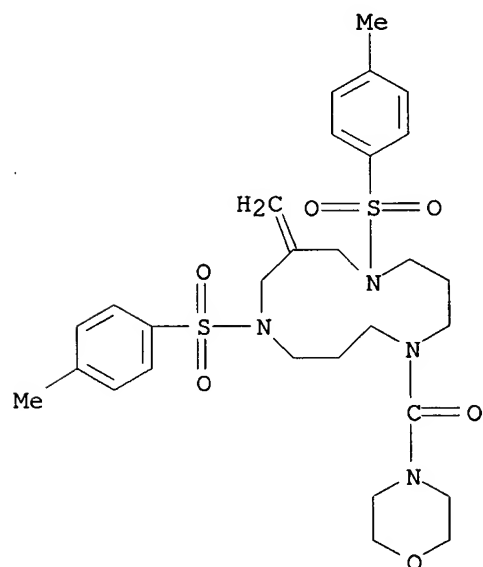
RN 881693-41-0 CAPLUS

CN 1,5,9-Triazacyclododecane-1-carboxamide, N,N-dimethyl-7-methylene-5,9-bis[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)



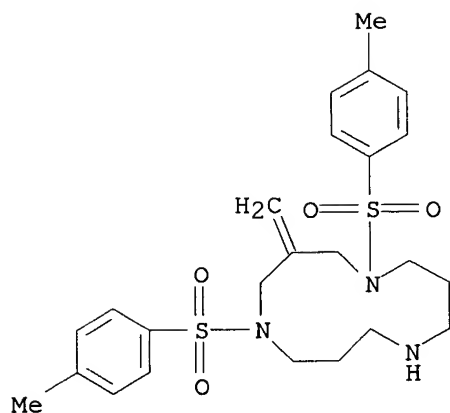
RN 881693-42-1 CAPLUS

CN 1,5,9-Triazacyclododecane, 3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]-9-(4-morpholinylcarbonyl)- (9CI) (CA INDEX NAME)



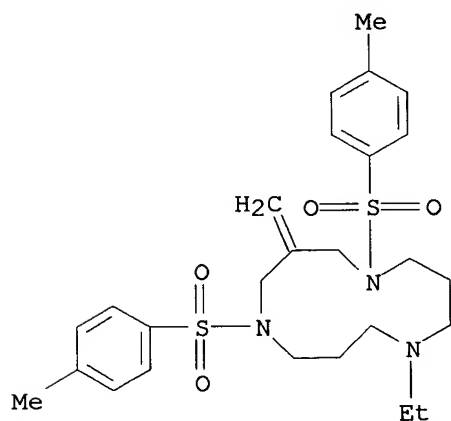
RN 881693-50-1 CAPLUS

CN 1,5,9-Triazacyclododecane, 3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]-, dihydrochloride (9CI) (CA INDEX NAME)



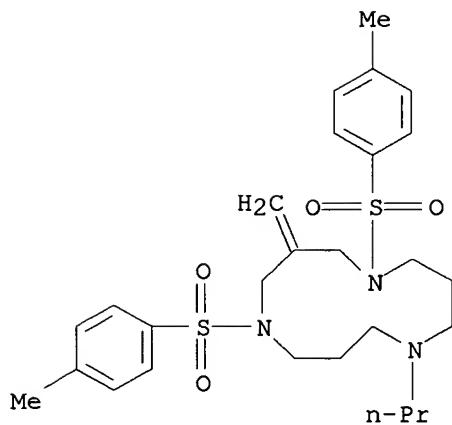
● 2 HCl

RN 881693-51-2 CAPLUS
 CN 1,5,9-Triazacyclododecane, 9-ethyl-3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

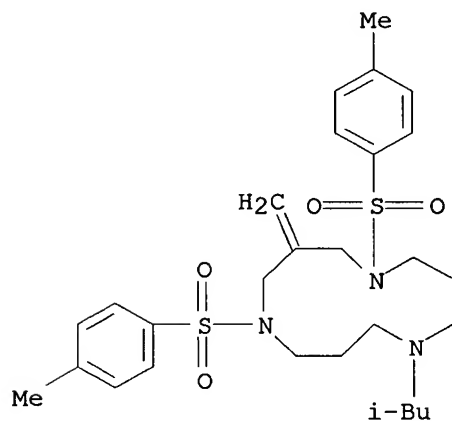
RN 881693-52-3 CAPLUS
 CN 1,5,9-Triazacyclododecane, 3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]-9-propyl-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 881693-53-4 CAPLUS

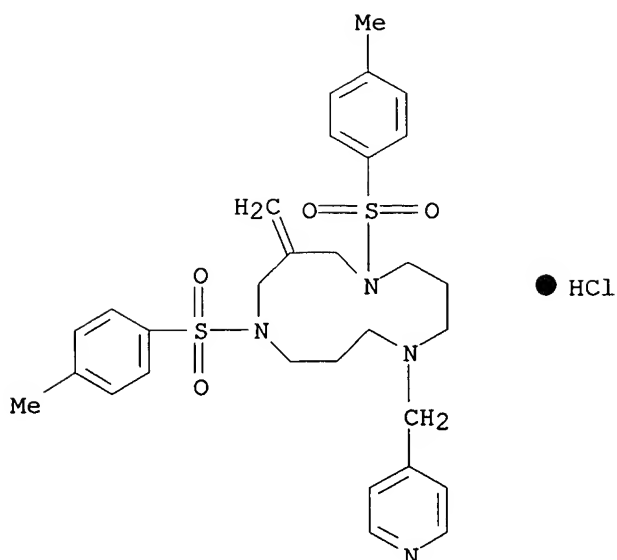
CN 1,5,9-Triazacyclododecane, 3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]-9-(2-methylpropyl)-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

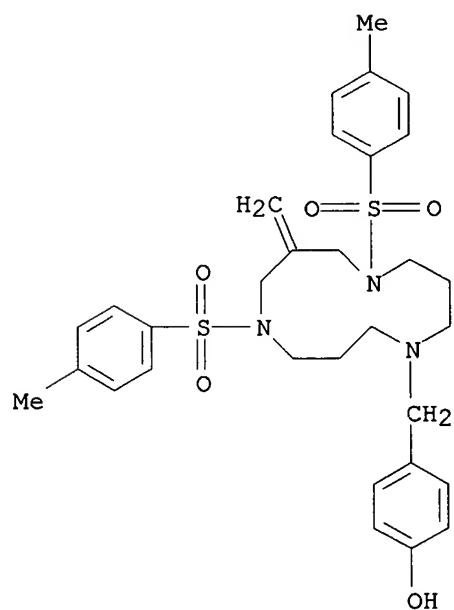
RN 881693-60-3 CAPLUS

CN 1,5,9-Triazacyclododecane, 3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]-9-(4-pyridinylmethyl)-, monohydrochloride (9CI) (CA INDEX NAME)



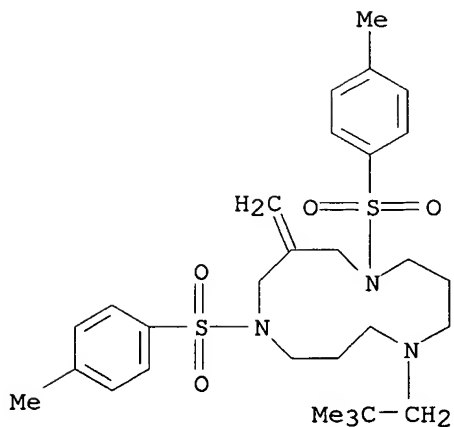
RN 881693-61-4 CAPLUS

CN 1,5,9-Triazacyclododecane, 9-[(4-hydroxyphenyl)methyl]-3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)



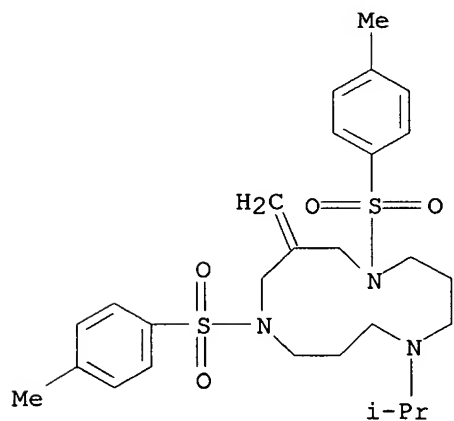
RN 881693-63-6 CAPLUS

CN 1,5,9-Triazacyclododecane, 9-(2,2-dimethylpropyl)-3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]-, monohydrochloride (9CI) (CA INDEX NAME)



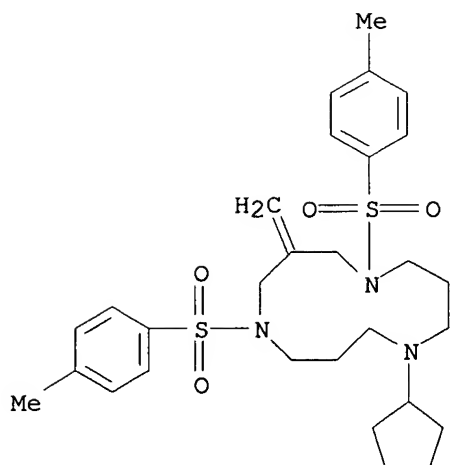
● HCl

RN 881693-64-7 CAPLUS
 CN 1,5,9-Triazacyclododecane, 3-methylene-9-(1-methylethyl)-1,5-bis[(4-methylphenyl)sulfonyl]-, monohydrochloride (9CI) (CA INDEX NAME)



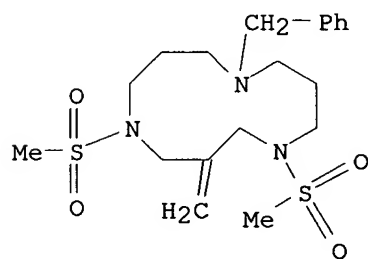
● HCl

RN 881693-65-8 CAPLUS
 CN 1,5,9-Triazacyclododecane, 9-cyclopentyl-3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]-, monohydrochloride (9CI) (CA INDEX NAME)



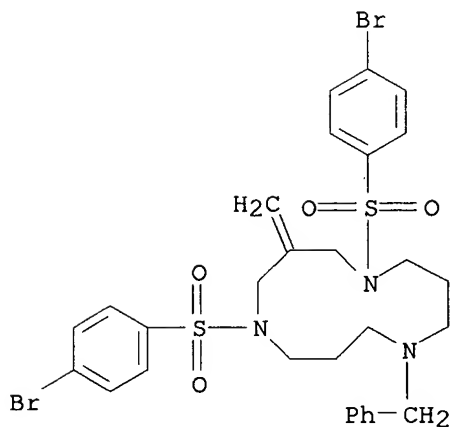
● HCl

RN 881693-66-9 CAPLUS
 CN 1,5,9-Triazacyclododecane, 3-methylene-1,5-bis(methylsulfonyl)-9-(phenylmethyl)-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

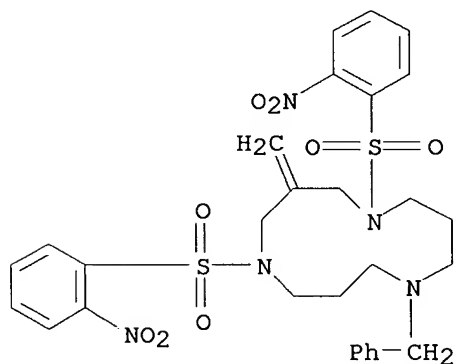
RN 881693-70-5 CAPLUS
 CN 1,5,9-Triazacyclododecane, 1,5-bis[(4-bromophenyl)sulfonyl]-3-methylene-9-(phenylmethyl)-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 881693-73-8 CAPLUS

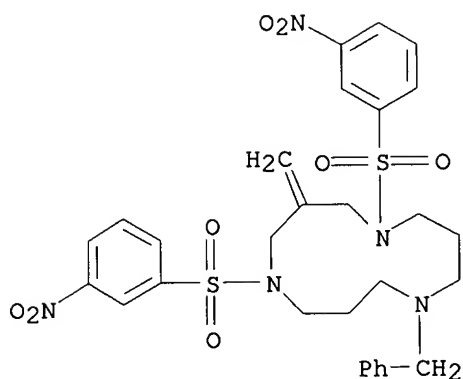
CN 1,5,9-Triazacyclododecane, 3-methylene-1,5-bis[(2-nitrophenyl)sulfonyl]-9-(phenylmethyl)-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 881693-75-0 CAPLUS

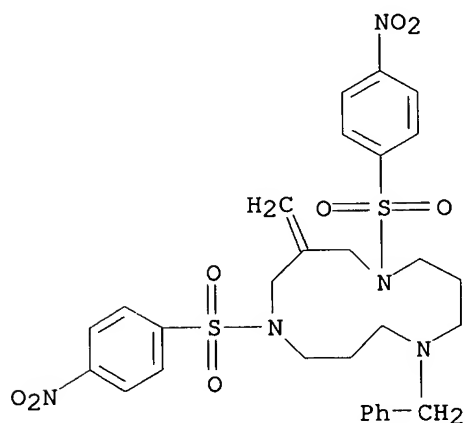
CN 1,5,9-Triazacyclododecane, 3-methylene-1,5-bis[(3-nitrophenyl)sulfonyl]-9-(phenylmethyl)-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 881693-77-2 CAPLUS

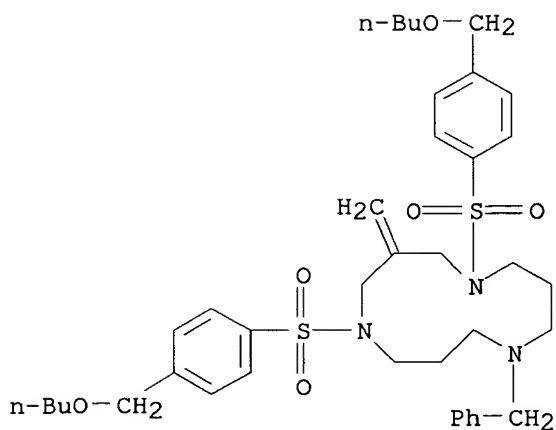
CN 1,5,9-Triazacyclododecane, 3-methylene-1,5-bis[(4-nitrophenyl)sulfonyl]-9-(phenylmethyl)-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 881693-83-0 CAPLUS

CN 1,5,9-Triazacyclododecane, 1,5-bis[[4-(butoxymethyl)phenyl]sulfonyl]-3-methylene-9-(phenylmethyl)-, monohydrochloride (9CI) (CA INDEX NAME)



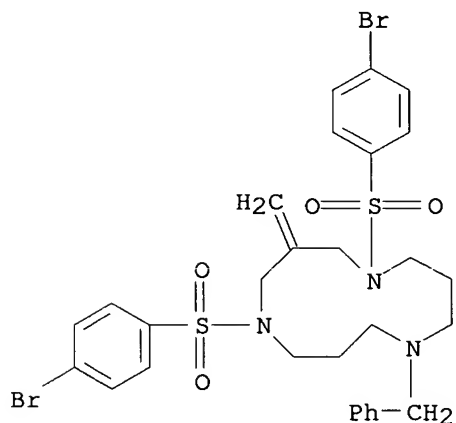
● HCl

IT 471867-02-4P

RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of (methylene)bis[(bromophenyl)sulfonyl]-1,5,9-triazacyclododecane (ASPB-127) and study of its crystal and mol. structures)

RN 471867-02-4 CAPLUS

CN 1,5,9-Triazacyclododecane, 1,5-bis[(4-bromophenyl)sulfonyl]-3-methylene-9-(phenylmethyl)- (9CI) (CA INDEX NAME)



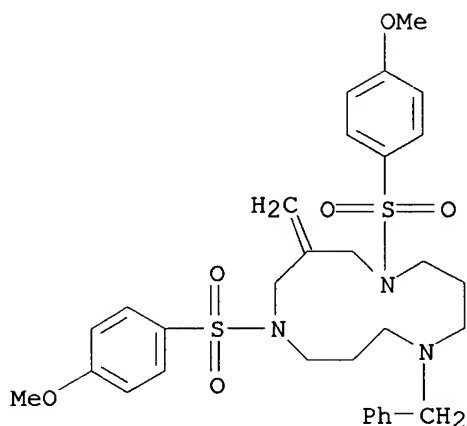
IT 881693-71-6P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation of (methylene)bis[(bromophenyl)sulfonyl]-1,5,9-triazacyclododecane (KKD-023), study of its crystal and mol. structures and its CD4 down-modulating structure-activity relationship study with CADA analogs)

RN 881693-71-6 CAPLUS

CN 1,5,9-Triazacyclododecane, 1,5-bis[(4-methoxyphenyl)sulfonyl]-3-methylene-

9-(phenylmethyl)- (9CI) (CA INDEX NAME)



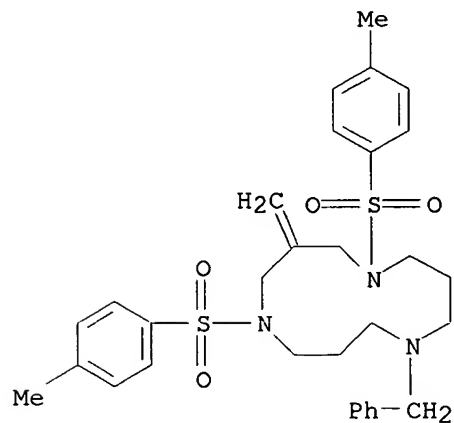
IT 182316-44-5P, CADA

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of (methylene)bis[(methylphenyl)sulfonyl](benzyl)-1,5,9-triazacyclododecane (CADA) and study of its crystal and mol. structures)

RN 182316-44-5 CAPLUS

CN 1,5,9-Triazacyclododecane, 3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]-9-(phenylmethyl)- (9CI) (CA INDEX NAME)



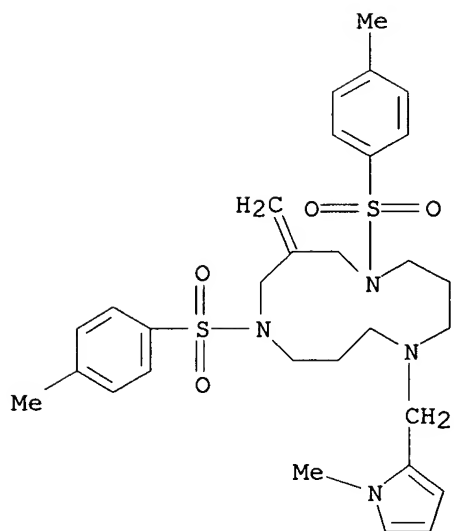
IT 881693-35-2P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)

(preparation of (methylene)bis[(methylphenyl)sulfonyl](pyrazolylmethyl)-1,5,9-triazacyclododecane (CADA analog) and study of its crystal and mol. structures)

RN 881693-35-2 CAPLUS

CN 1,5,9-Triazacyclododecane, 3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]-9-[(1-methyl-1H-pyrrol-2-yl)methyl]- (9CI) (CA INDEX NAME)



REFERENCE COUNT:

47

THERE ARE 47 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

10/680,076

~~120~~ ANSWER 4 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2005:704359 CAPLUS

DOCUMENT NUMBER: 143:326191

TITLE: An unusual substitution reaction directed by an intramolecular re-arrangement

AUTHOR(S): Parenty, Alexis D. C.; Smith, Louise V.; Cronin, Leroy

CORPORATE SOURCE: Department of Chemistry, University of Glasgow, Glasgow, G12 8QQ, UK

SOURCE: Tetrahedron (2005), 61(35), 8410-8418

CODEN: TETRAE; ISSN: 0040-4020

PUBLISHER: Elsevier B.V.

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 143:326191

AB Secondary amines and thiols undertake a substitution reaction on the side chain of 2-bromoethylpyridinium derivs. directed by an intramol. rearrangement. Exptl. investigations strongly indicate that the reaction is initiated by an alpha addition of the nucleophile onto the iminium moiety of the N-heteroarom. cation, followed by a cyclization and an oxidative ring opening. This novel substitution process is able to occur with less reactive nucleophiles that would not undergo conventional substitution with isolated bromoethyl moieties.

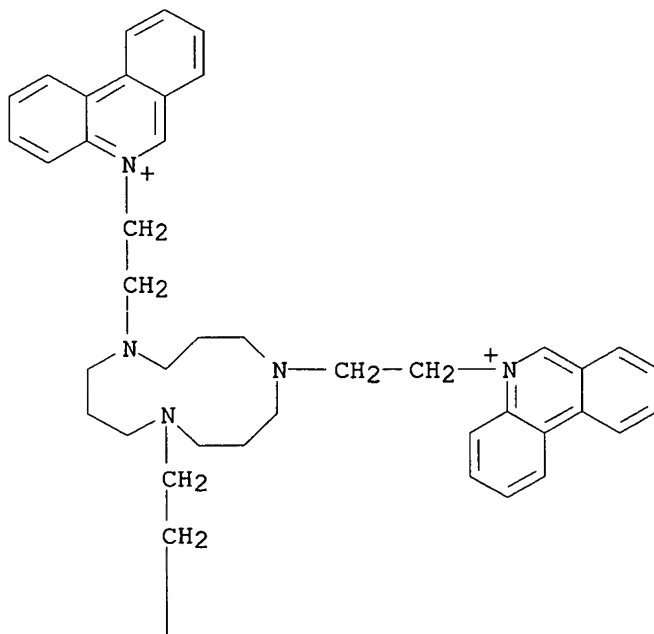
IT 854516-25-9P

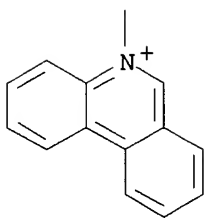
RL: SPN (Synthetic preparation); PREP (Preparation)
(rearrangement in the amination of fluoroethylphenanthridine)

RN 854516-25-9 CAPLUS

CN Phenanthridinium, 5,5',5''-(1,5,9-triazacyclododecane-1,5,9-triyltri-2,1-ethanediyl)tris-, tribromide (9CI) (CA INDEX NAME)

PAGE 1-A





● 3 Br⁻

REFERENCE COUNT:

28

THERE ARE 28 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

10/680,076

~~180~~ ANSWER 5 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2005:523454 CAPLUS

DOCUMENT NUMBER: 143:59981

TITLE: Preparation imidazophenanthridiniums and related compounds as anticancer agents

INVENTOR(S): Parenty, Alexis; Cronin, Leroy; Brown, Robert

PATENT ASSIGNEE(S): The University Court of the University of Glasgow, UK

SOURCE: PCT Int. Appl., 122 pp.

CODEN: PIXXD2

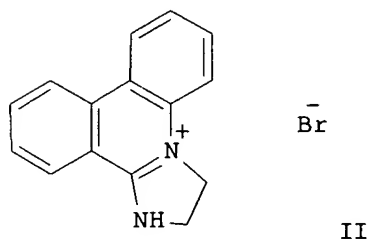
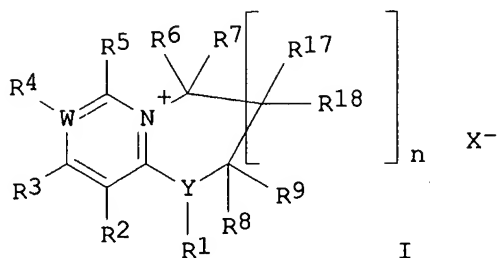
DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005054241	A2	20050616	WO 2004-GB5004	20041126
WO 2005054241	A3	20050728		
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			
RW:	BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
EP 1692130	A2	20060823	EP 2004-798693	20041126
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK, IS			
PRIORITY APPLN. INFO.:			GB 2003-27524	A 20031126
			WO 2004-GB5004	W 20041126
OTHER SOURCE(S):	CASREACT 143:59981; MARPAT 143:59981			
GI				



AB Title compds. I [$n = 0-3$; further details on n are given.; $W = C, N$; $Y = N, O, S$; $R_1 = H$, (un)substituted alkyl, (un)substituted cycloalkyl, etc.; $R_2, R_3, R_4, R_5 = \text{halo, hydroxy, oxo, etc.}$; $R_6, R_7 = H, \text{halo, hydroxy, etc.}$; $R_8, R_9 = H, \text{halo, hydroxy, etc.}$; $R_{17}, R_{18} = H, \text{halo, hydroxy, etc.}$; $X = \text{anion moiety}$] were prepared For example, bromoethylation of phenanthridine followed by treatment with 35% ammonia in water afforded compound II. In cytotoxicity assays, the IC_{50} value of compound II was $1.56 \mu M$. Compds. I are claimed useful as anticancer agents, DNA binding agents, etc.

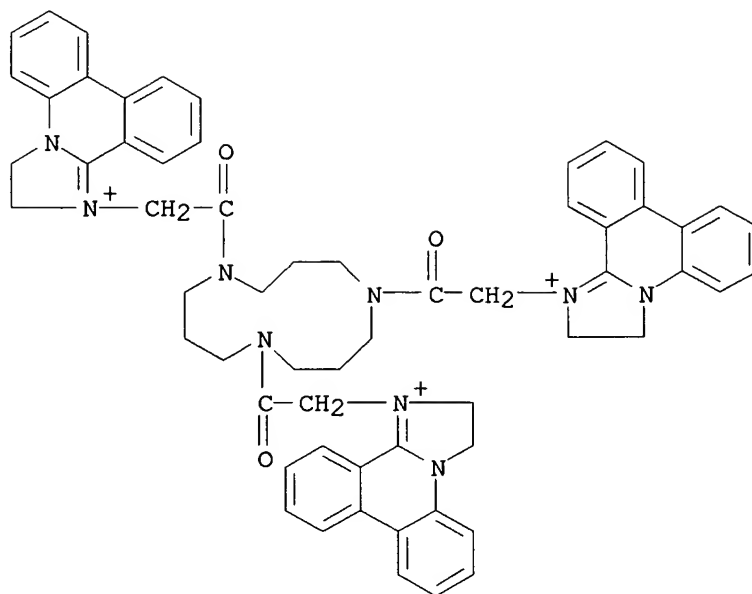
IT 854516-15-7P 854516-25-9P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation imidazophenanthridiniums and related compds. as anticancer agents)

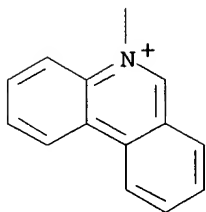
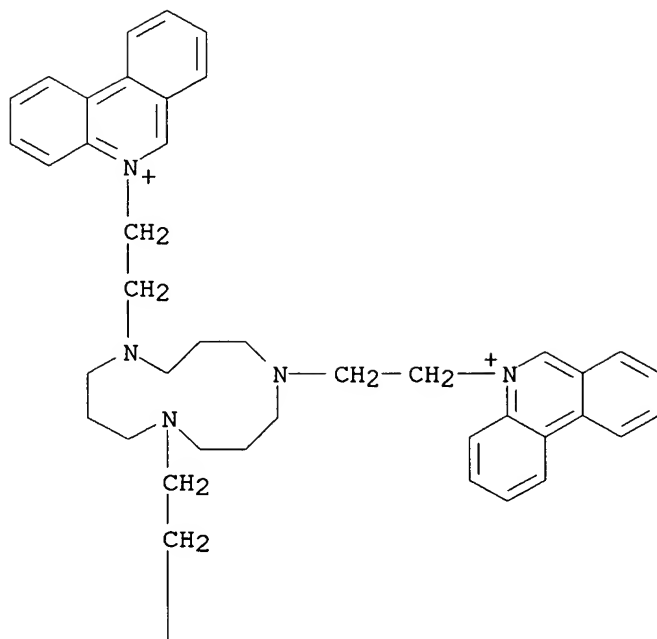
RN 854516-15-7 CAPLUS

CN Imidazo[1,2-f]phenanthridinium, 1,1',1''-[1,5,9-triazacyclododecane-1,5,9-triyl]tris(2-oxo-2,1-ethanediyl)]tris[2,3-dihydro-, tribromide (9CI) (CA INDEX NAME)



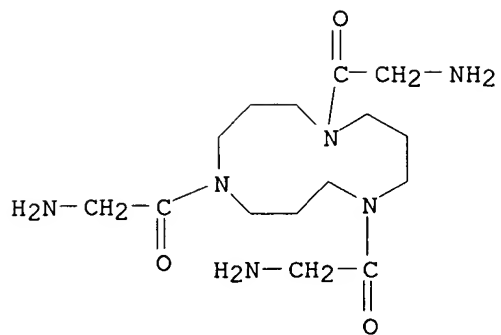
● 3 Br⁻

RN 854516-25-9 CAPLUS
 CN Phenanthridinium, 5,5',5''-(1,5,9-triazacyclododecane-1,5,9-triyltri-2,1-ethanediyl)tris-, tribromide (9CI) (CA INDEX NAME)



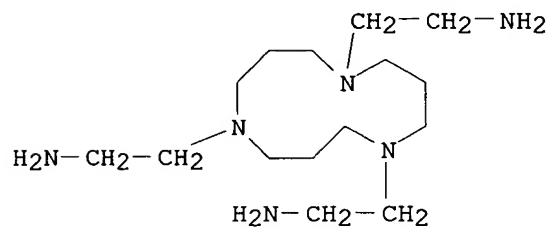
● 3 Br⁻

IT 854276-73-6 854276-74-7
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (spacer for trimer; preparation imidazophenanthridiniums and related compds.
 as anticancer agents)
 RN 854276-73-6 CAPLUS
 CN 1,5,9-Triazacyclododecane, 1,5,9-tris(aminoacetyl)- (9CI) (CA INDEX NAME)



RN 854276-74-7 CAPLUS

CN 1,5,9-Triazacyclododecane-1,5,9-triethanamine (9CI) (CA INDEX NAME)



130 ANSWER 6 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2005:461020 CAPLUS

DOCUMENT NUMBER: 143:153359

TITLE: Synthesis of azamacrocycles via a Mitsunobu reaction

AUTHOR(S): Hovinen, Jari; Sillanpää, Reijo

CORPORATE SOURCE: PerkinElmer Life and Analytical Sciences, Turku, FIN-20101, Finland

SOURCE: Tetrahedron Letters (2005), 46(25), 4387-4389

CODEN: TELEAY; ISSN: 0040-4039

PUBLISHER: Elsevier B.V.

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 143:153359

AB Reaction of protected diethylenetriamine and 2-substituted propane-1,3-diols in dry THF in the presence of triphenylphosphine and diisopropyl azodicarboxylate gives the corresponding protected 9-substituted 1,4,7-triazacyclododecanes. The Mitsunobu reaction was also used in the preparation of 3-substituted 1,5,9-triazacyclododecanes and macrocyclic pyridine derivs.

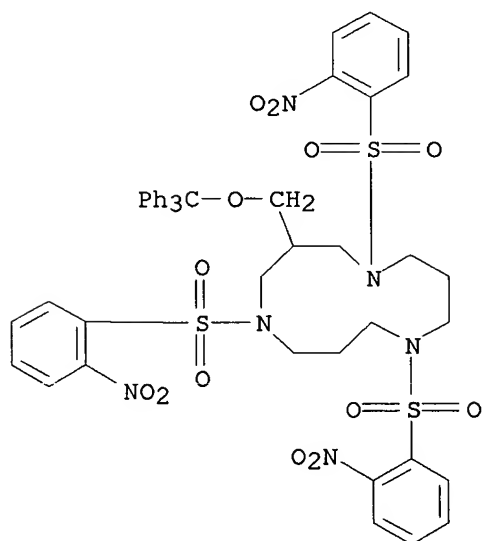
IT 859502-16-2P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of functionalized triazacyclododecanes, triazacyclododecanes and analogs via Mitsunobu reaction of protected dialkylenetriamines with diols)

RN 859502-16-2 CAPLUS

CN 1,5,9-Triazacyclododecane, 1,5,9-tris[(2-nitrophenyl)sulfonyl]-3-[(triphenylmethoxy)methyl]- (9CI) (CA INDEX NAME)



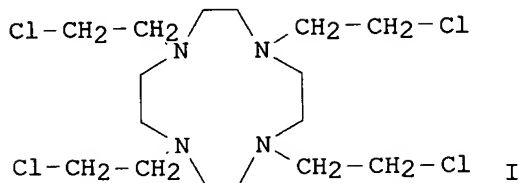
REFERENCE COUNT:

22

THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

130 ANSWER 7 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2005:202831 CAPLUS
 DOCUMENT NUMBER: 142:456249
 TITLE: Synthesis of novel DNA cross-linking antitumour agents based on polyazamacrocycles
 AUTHOR(S): Parker, Laurie L.; Anderson, Fiona M.; O'Hare, C. Caroline; Lacy, Stephen M.; Bingham, John P.; Robins, David J.; Hartley, John A.
 CORPORATE SOURCE: Department of Chemistry, University of Glasgow, Glasgow, G12 8QQ, UK
 SOURCE: Bioorganic & Medicinal Chemistry (2005), 13(7), 2389-2395
 CODEN: BMECEP; ISSN: 0968-0896
 PUBLISHER: Elsevier Ltd.
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 142:456249
 GI



AB The authors are seeking to develop more effective alkylating agents as antitumor agents. In previous work conformationally restricted nitrogen mustards were synthesized containing piperidine or pyrrolidine rings. The free bases were designed to be bifunctional alkylating agents via aziridinium ion formation and the effects of varying the distances between the two alkylating sites were studied. Some efficient crosslinkers of naked DNA were prepared but few of these compds. exhibited significant cytotoxicity in human tumor cells in vitro. The authors have extended this work by making tri- and tetra-azamacrocyclic compds. containing two to four potential alkylating sites. Most of these compds. were powerful DNA alkylating agents and showed cytotoxicity (IC₅₀ values 6-100 μ M) comparable with chlorambucil (45 μ M) and melphalan (8.5 μ M). In particular the cyclen derivative I was more than 104 times more effective at crosslinking DNA (XL₅₀ \ll 10 nM) than chlorambucil (XL₅₀ 100 μ M), and showed significant cytotoxicity in human tumor cells in vitro.

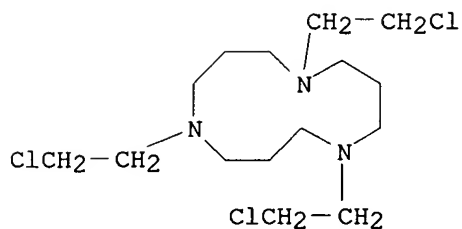
IT 850894-95-0P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

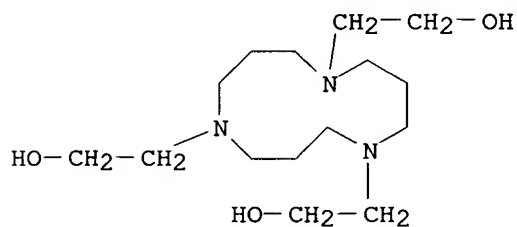
(synthesis of novel DNA crosslinking antitumor agents based on polyazamacrocycles)

RN 850894-95-0 CAPLUS

CN 1,5,9-Triazacyclododecane, 1,5,9-tris(2-chloroethyl)- (9CI) (CA INDEX NAME)



IT 850895-04-4P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (synthesis of novel DNA crosslinking antitumor agents based on
 polyazamacrocycles)
 RN 850895-04-4 CAPLUS
 CN 1,5,9-Triazacyclododecane-1,5,9-triethanol (9CI) (CA INDEX NAME)



REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

130 ANSWER 8 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2004:1079564 CAPLUS

DOCUMENT NUMBER: 142:232412

TITLE: CADA, a novel CD4-targeted HIV inhibitor, is synergistic with various anti-HIV drugs in vitro

AUTHOR(S): Vermeire, Kurt; Princen, Katrien; Hatse, Sigrid; de Clercq, Erik; Dey, Kaka; Bell, Thomas W.; Schols, Dominique

CORPORATE SOURCE: Rega Institute for Medical Research, Katholieke Universiteit Leuven, Louvain, B-3000, Belg.

SOURCE: AIDS (London, United Kingdom) (2004), 18(16), 2115-2125

CODEN: AIDSET; ISSN: 0269-9370

PUBLISHER: Lippincott Williams & Wilkins

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Objective: To evaluate the anti-HIV-1 activity of the cyclotriazadisulfonamide CADA against primary isolates in vitro and the combination of CADA with approved anti-HIV drugs for potential synergy. Methods: Peripheral blood mononuclear cells (PBMC) were treated with CADA and infected with 16 different clin. isolates. After 8 days of infection, the median inhibitory concentration (IC50) was calculated from the p24 viral antigen

content in the supernatant. MT-4 cells were infected with HIV-1NL4.3 and then cultured with CADA or other antiretroviral drugs (i.e., several reverse transcriptase, protease and entry inhibitors), alone and in combination. After 4 days, IC50 was determined for the various drugs in replicate assays. Anal. of combined effects was performed using the median effect principle (CalcuSyn; Biosoft). Results: The entry inhibitor CADA exerted a potent and consistent anti-HIV-1 activity against a wide range of R5, R5/X4 and X4 primary isolates in PBMC. From the two-drug studies, combination indexes showed synergy between CADA and reverse transcriptase inhibitors (zidovudine, stavudine, lamivudine, zalcitabine, didanosine, abacavir, tenofovir, nevirapine, delavirdine and efavirenz), and protease inhibitors (lopinavir, saquinavir, indinavir, nelfinavir, amprenavir and ritonavir). In addition, the combination of CADA with the gp41 fusion inhibitor T-20 (enfuvirtide), the CXCR4 antagonist AMD3100 and the gp120-specific interacting plant lectins from Galanthus nivalis (GNA) and Hippeastrum hybrid (HHA) also resulted in a synergistic inhibition. Conclusions: Compds. that can specifically downmodulate the CD4 receptor in PBMC have broad-spectrum anti-HIV activity against primary isolates and act synergistically when used in conjunction with currently available antiretroviral drugs. They deserve further study as potential candidate anti-HIV drugs.

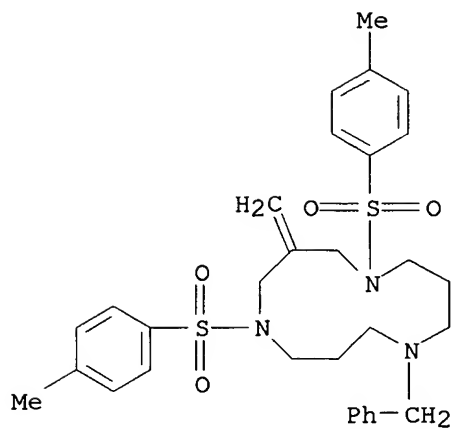
IT 182316-44-5, CADA

RL: DMA (Drug mechanism of action); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(CD4-downmodulating compound CADA with potent anti-HIV-1 activity against R5, R5/X4 and X4 primary isolates in PBMC and showed favorable in vitro interaction and synergistic action with antiretroviral agent like RT, protease, entry inhibitor)

RN 182316-44-5 CAPLUS

CN 1,5,9-Triazacyclododecane, 3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]-9-(phenylmethyl)- (9CI) (CA INDEX NAME)



REFERENCE COUNT:

65

THERE ARE 65 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L30 ANSWER 9 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2003:996287 CAPLUS

DOCUMENT NUMBER: 140:235998

TITLE: Preparation of Aza-Crown-Functionalized 2'-O-Methyl
Oligoribonucleotides, Potential Artificial RNasesAUTHOR(S): Niittymaeki, Teija; Kaukinen, Ulla; Virta, Pasi;
Mikkola, Satu; Loennberg, HarriCORPORATE SOURCE: Department of Chemistry, University of Turku, Turku,
FIN-20014, Finland

SOURCE: Bioconjugate Chemistry (2004), 15(1), 174-184

CODEN: BCCHE; ISSN: 1043-1802

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB An improved synthesis for 3-(3-aminopropyl)- and 3-(3-mercaptopropyl)-1,5,9-triazacyclododecane has been developed and alternative methods for their conjugation to oligonucleotides have been described. Accordingly, the 3-aminopropyl aza-crown and its N-(3-aminopropanoyl)-3-aminopropyl analog have been tethered to the 3'-terminus of a 2'-O-methyloligoribonucleotide by aminolytic cleavage of the thio-ester linker utilized for the chain assembly. Studies on a monomeric model compound verify that the reaction proceeds solely by the attack of the primary amino group. 5'-Conjugation has been achieved by introducing a 2-benzylthio-2-oxoethyl group to the 5'-terminus as a phosphoramidite reagent and cleaving the thioester bond with the 3-aminopropyl aza-crown. For intrachain conjugation, a phosphoramidite reagent derived from 1-deoxy-1-(2-benzylthio-2-oxoethyl)- β -D-erythro-pentofuranose has been inserted in a desired position within the chain and subjected to on-support aminolysis with the 3-aminopropyl aza-crown or its N-(3-aminopropanoyl)-3-aminopropyl and N-(6-aminohexanoyl)-3-aminopropyl analogs. The 3-mercaptopropyl-derivatized aza-crown has been tethered by a disulfide bond to a 3'-(3-mercaptoalkyl)phosphate-tailed oligonucleotide. The 3'- and intrachain-tethered conjugates have been shown to cleave as their Zn(II) chelate complementary oligoribonucleotide sequences.

IT 663198-88-7P 663198-89-8P 663198-90-1P

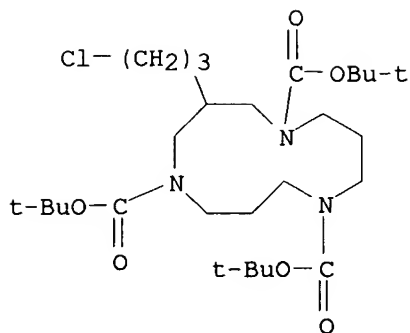
663198-91-2P 663198-93-4P 663198-94-5P

663198-96-7P 663198-97-8P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)(preparation of aza-crown-functionalized 2'-O-Me oligoribonucleotides as
potential artificial RNases)

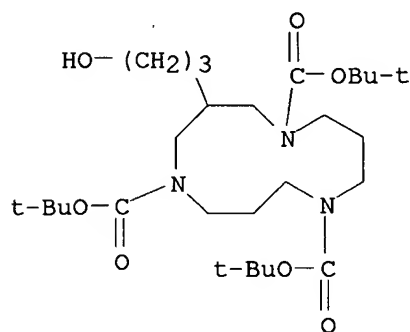
RN 663198-88-7 CAPLUS

CN 1,5,9-Triazacyclododecane-1,5,9-tricarboxylic acid, 3-(3-chloropropyl)-,
tris(1,1-dimethylethyl) ester (9CI) (CA INDEX NAME)



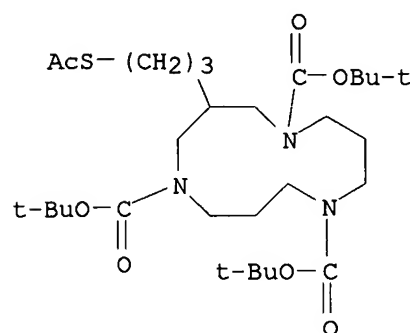
RN 663198-89-8 CAPLUS

CN 1,5,9-Triazacyclododecane-1,5,9-tricarboxylic acid, 3-(3-hydroxypropyl)-, tris(1,1-dimethylethyl) ester (9CI) (CA INDEX NAME)



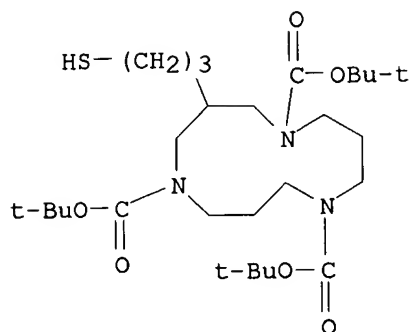
RN 663198-90-1 CAPLUS

CN 1,5,9-Triazacyclododecane-1,5,9-tricarboxylic acid, 3-[3-(acetylthio)propyl]-, tris(1,1-dimethylethyl) ester (9CI) (CA INDEX NAME)



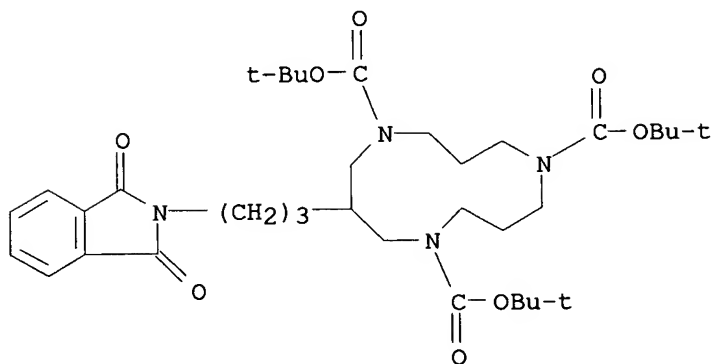
RN 663198-91-2 CAPLUS

CN 1,5,9-Triazacyclododecane-1,5,9-tricarboxylic acid, 3-(3-mercaptopropyl)-, tris(1,1-dimethylethyl) ester (9CI) (CA INDEX NAME)



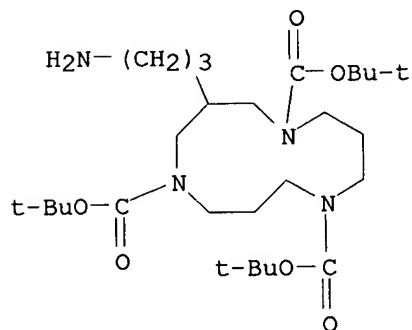
RN 663198-93-4 CAPLUS

CN 1,5,9-Triazacyclododecane-1,5,9-tricarboxylic acid, 3-[3-(1,3-dihydro-1,3-dioxo-2H-isoindol-2-yl)propyl]-, tris(1,1-dimethylethyl) ester (9CI) (CA INDEX NAME)



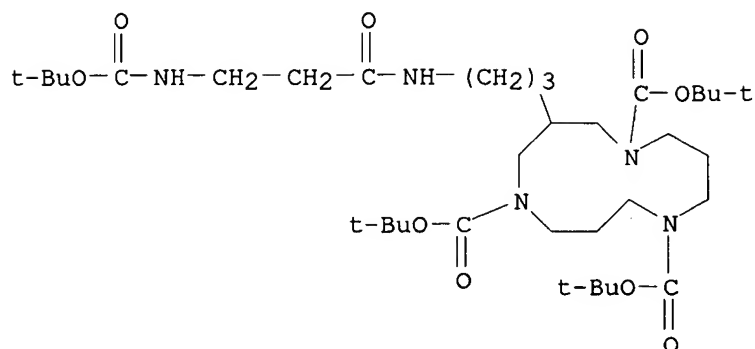
RN 663198-94-5 CAPLUS

CN 1,5,9-Triazacyclododecane-1,5,9-tricarboxylic acid, 3-(3-aminopropyl)-, tris(1,1-dimethylethyl) ester (9CI) (CA INDEX NAME)



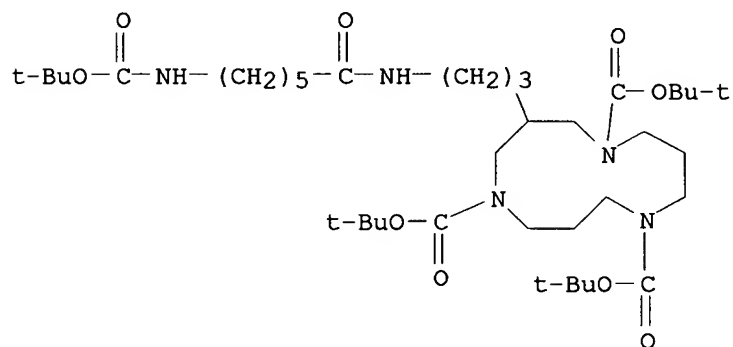
RN 663198-96-7 CAPLUS

CN 1,5,9-Triazacyclododecane-1,5,9-tricarboxylic acid, 3-[3-[[3-[[[(1,1-dimethylethoxy)carbonyl]amino]-1-oxopropyl]amino]propyl]-, tris(1,1-dimethylethyl) ester (9CI) (CA INDEX NAME)



RN 663198-97-8 CAPLUS

CN 1,5,9-Triazacyclododecane-1,5,9-tricarboxylic acid, 3-[[3-[[6-[[1,1-dimethylethoxy]carbonyl]amino]-1-oxohexyl]amino]propyl]-, tris(1,1-dimethylethyl) ester (9CI) (CA INDEX NAME)



REFERENCE COUNT:

56

THERE ARE 56 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

~~150~~ ANSWER 10 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2003:727508 CAPLUS

DOCUMENT NUMBER: 139:350441

TITLE: Syntheses, Conformations, and Basicities of Bicyclic Triamines

AUTHOR(S): Bell, Thomas W.; Choi, Heung-Jin; Harte, William; Drew, Michael G. B.

CORPORATE SOURCE: Department of Chemistry, University of Nevada, Reno, NV, 89557-0020, USA

SOURCE: Journal of the American Chemical Society (2003), 125(40), 12196-12210

CODEN: JACSAT; ISSN: 0002-7863

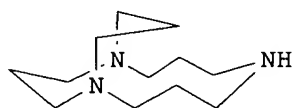
PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

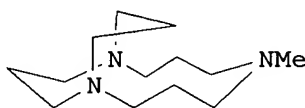
LANGUAGE: English

OTHER SOURCE(S): CASREACT 139:350441

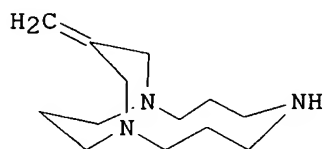
GI



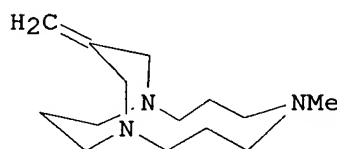
XII



XIII



XV



XVI

AB The multistep syntheses of several bicyclic triamines are described, all of which have an imbedded 1,5,9-triazacyclododecane ring. In 1,5,9-triazabicyclo[7.3.3]pentadecanes 12, 13, 15, and 16, (XII, XIII, XV, and XVI, resp.) two nitrogens are bridged by three carbons. The monoprotinated forms of these triamines are highly stabilized by a hydrogen-bonded network involving the bridge and both bridgehead nitrogens, producing a difference of more than 8 pKa units in acidities of their monoprotinated and diprotinated forms. The one- and zero-carbon bridges in 1,5,9-triazabicyclo[9.1.1]tridecane and 7-methyl-1,5,9-triazabicyclo[5.5.0]dodecane do not enhance the stabilities of their monoprotinated forms. X-ray crystal structures and computational studies of 12·HI and 16·HI reveal similar, but somewhat weaker, hydrogen-bonded networks, relative to 15·HI. The activation free energies for conformational inversion of 13·HI (14.4 ± 0.2 kcal/mol), 16·HI (15.0 ± 0.1 kcal/mol) and 16 (8.8 ± 0.3 kcal/mol) were measured by variable-temperature ^1H and ^{13}C NMR spectroscopy. These exptl. barriers give an estimate of 6.2 kcal/mol for the strength of the bifurcated hydrogen bond between the bridge nitrogen and cavity proton in 16·HI. Computational studies support the hypothesis that N-inversion occurs in an open conformation, leading to an estimate of 10.32 kcal/mol for the enthalpy of the bifurcated hydrogen bond in 16·HI in the gas phase. Safety: explosion hazard; air must be completely replaced by H_2 in Parr apparatus before hydrogenation of bis(2-cyanoethyl)benzylamine.

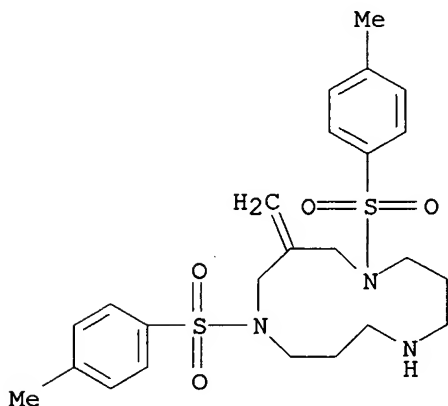
IT 182316-06-9P 182316-12-7P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

(Reactant or reagent)

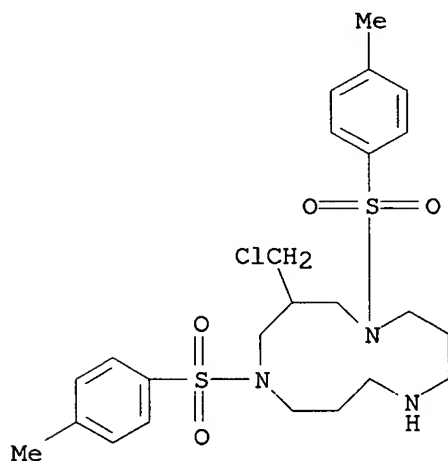
(attempted cyclization; syntheses, conformations, and basicities of bicyclic triamines containing embedded 1,5,9-triazacyclododecane ring)

RN 182316-06-9 CAPLUS

CN 1,5,9-Triazacyclododecane, 3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]-
(9CI) (CA INDEX NAME)

RN 182316-12-7 CAPLUS

CN 1,5,9-Triazacyclododecane, 3-(chloromethyl)-1,5-bis[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)



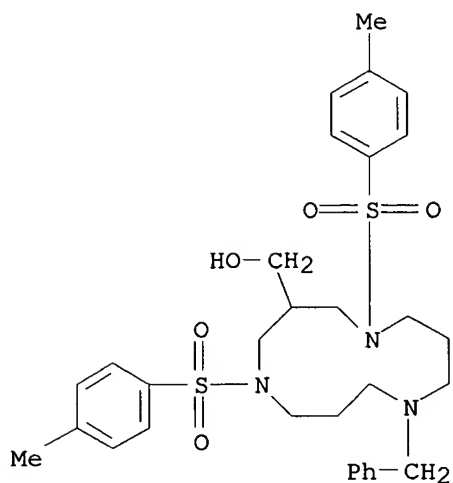
IT 182316-08-1P 182316-17-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)

(chlorination; syntheses, conformations, and basicities of bicyclic triamines containing embedded 1,5,9-triazacyclododecane ring)

RN 182316-08-1 CAPLUS

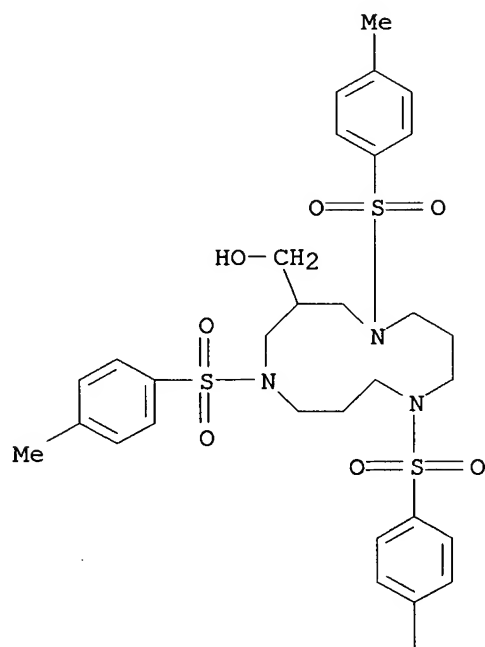
CN 1,5,9-Triazacyclododecane-3-methanol, 1,5-bis[(4-methylphenyl)sulfonyl]-9-
(phenylmethyl)- (9CI) (CA INDEX NAME)



RN 182316-17-2 CAPLUS

CN 1,5,9-Triazacyclododecane-3-methanol, 1,5,9-tris[(4-methylphenyl)sulfonyl]-
(9CI) (CA INDEX NAME)

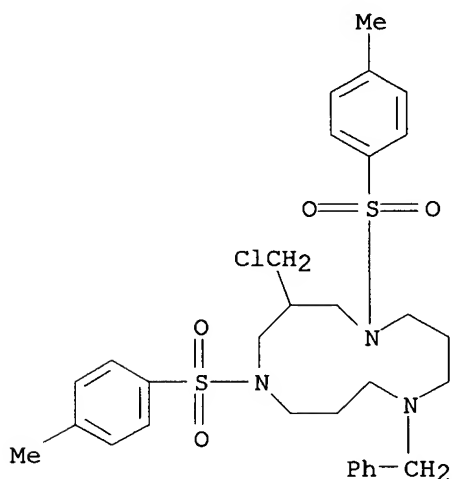
PAGE 1-A



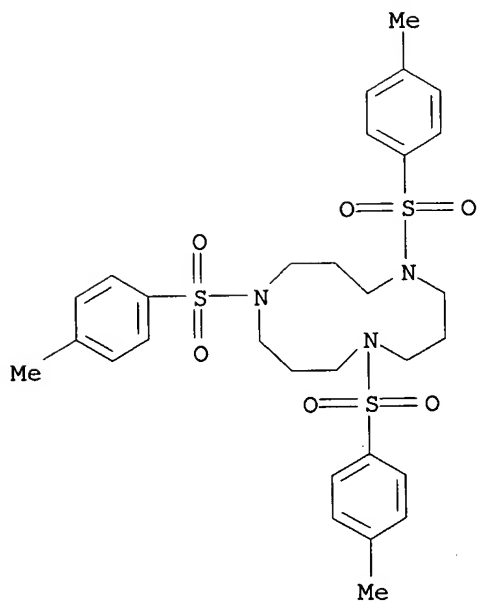
PAGE 2-A

Me

IT 182316-10-5P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (deprotection; syntheses, conformations, and basicities of bicyclic
 triamines containing embedded 1,5,9-triazacyclododecane ring)
 RN 182316-10-5 CAPLUS
 CN 1,5,9-Triazacyclododecane, 3-(chloromethyl)-1,5-bis[(4-
 methylphenyl)sulfonyl]-9-(phenylmethyl)- (9CI) (CA INDEX NAME)

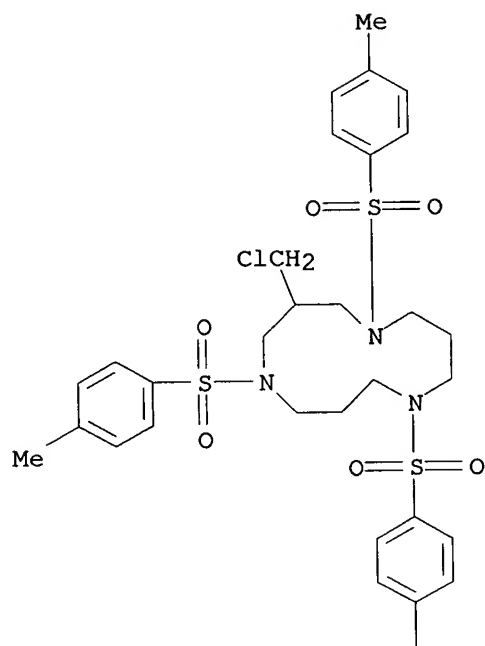


IT 35980-67-7P 182316-19-4P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (detosylation; syntheses, conformations, and basicities of bicyclic
 triamines containing embedded 1,5,9-triazacyclododecane ring)
 RN 35980-67-7 CAPLUS
 CN 1,5,9-Triazacyclododecane, 1,5,9-tris[(4-methylphenyl)sulfonyl]- (9CI)
 (CA INDEX NAME)



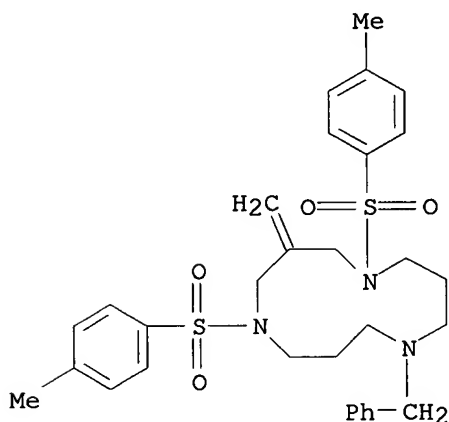
RN 182316-19-4 CAPLUS
 CN 1,5,9-Triazacyclododecane, 3-(chloromethyl)-1,5,9-tris[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)

PAGE 1-A

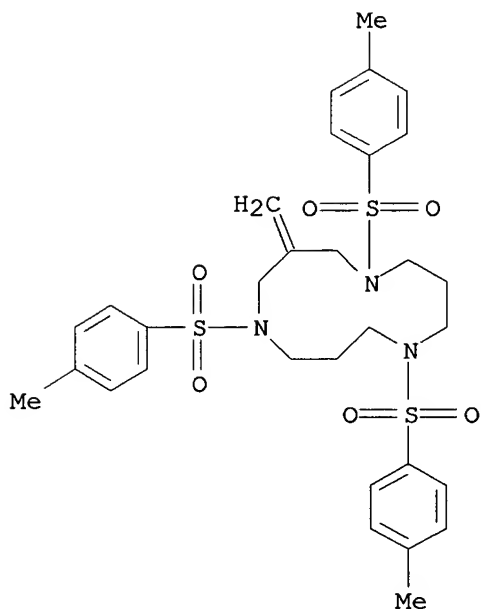


|
Me

IT 182316-44-5P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (hydroboration/oxidation and deprotection; syntheses, conformations, and
 basicities of bicyclic triamines containing embedded 1,5,9-
 triazacyclododecane ring)
 RN 182316-44-5 CAPLUS
 CN 1,5,9-Triazacyclododecane, 3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]-9-
 (phenylmethyl)- (9CI) (CA INDEX NAME)



IT 182316-15-0P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (hydroboration/oxidation; syntheses, conformations, and basicities of
 bicyclic triamines containing embedded 1,5,9-triazacyclododecane ring)
 RN 182316-15-0 CAPLUS
 CN 1,5,9-Triazacyclododecane, 3-methylene-1,5,9-tris[(4-
 methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)



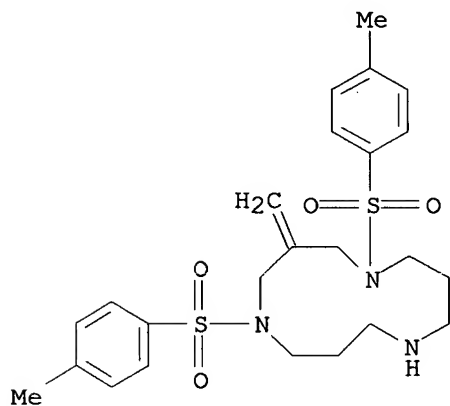
IT 392287-04-6P 618097-39-5P

RL: SPN (Synthetic preparation); PREP (Preparation)

(syntheses, conformations, and basicities of bicyclic triamines containing embedded 1,5,9-triazacyclododecane ring)

RN 392287-04-6 CAPLUS

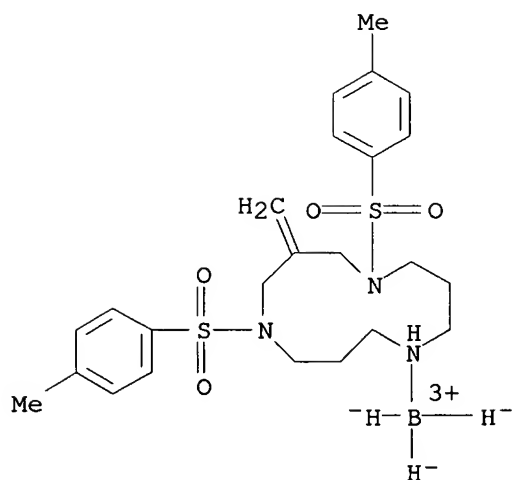
CN 1,5,9-Triazacyclododecane, 3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 618097-39-5 CAPLUS

CN Boron, trihydro[3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]-1,5,9-triazacyclododecane-κN9]-, (T-4)- (9CI) (CA INDEX NAME)



REFERENCE COUNT:

94

THERE ARE 94 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L30 ~~ANSWER~~ 11 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2003:3477 CAPLUS

DOCUMENT NUMBER: 139:30160

TITLE: The anti-HIV potency of cyclotriazadisulfonamide analogs is directly correlated with their ability to down-modulate the CD4 receptor

AUTHOR(S): Vermeire, Kurt; Bell, Thomas W.; Choi, Heung-Jin; Jin, Qi; Samala, Meinrado F.; Sodoma, Andrej; De Clercq, Erik; Schols, Dominique

CORPORATE SOURCE: Rega Institute for Medical Research, Katholieke Universiteit Leuven, Louvain, Belg.

SOURCE: Molecular Pharmacology (2003), 63(1), 203-210
CODEN: MOPMA3; ISSN: 0026-895X

PUBLISHER: American Society for Pharmacology and Experimental Therapeutics

DOCUMENT TYPE: Journal

LANGUAGE: English

AB 9-Benzyl-3-methylene-1,5-di-p-toluenesulfonyl-1,5,9-triazacyclododecane (CADA) has been identified as a novel antiviral lead compound with significant anti-human immunodeficiency virus and anti-human herpesvirus 7 activity. Surprisingly, this compound selectively decreased the expression of the CD4 glycoprotein, the primary receptor needed for the entry of both viruses. Herein, we describe the CD4 down-modulating and antiviral potencies of more than 25 CADA derivs. Flow cytometric evaluation of cellular CD4 receptor expression in T cells demonstrated the specific CD4 down-modulating capacity of the CADA derivs., with IC50 values similar to those obtained in the antiviral assays. The close correlation observed between the CD4 down-regulating and anti-HIV potencies of the CADA derivs. further points to CD4 receptor down-modulation as the primary mode of antiviral action for this group of compds.

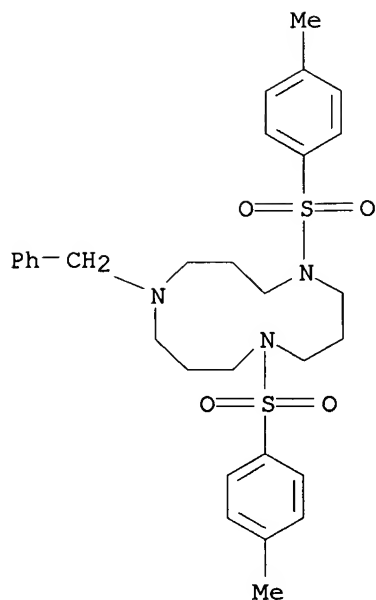
IT 164913-15-9 182316-08-1 182316-10-5
182316-15-0 182316-20-7 182316-30-9
182316-34-3 182316-44-5 471866-86-1
471866-87-2 471866-89-4 471866-90-7
471866-91-8 471866-92-9 471866-93-0
471866-94-1 471866-95-2 471866-96-3
471866-97-4 471866-98-5 471866-99-6
471867-00-2 471867-02-4 471867-03-5
471867-04-6 471867-05-7 471867-06-8
544430-76-4

RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(the anti-HIV potency of cyclotriazadisulfonamide analogs is directly correlated with their ability to down-modulate the CD4 receptor)

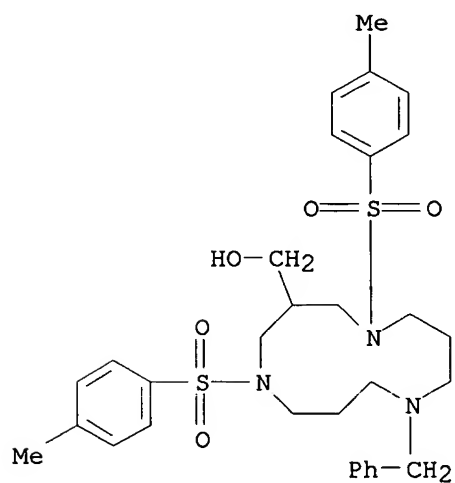
RN 164913-15-9 CAPLUS

CN 1,5,9-Triazacyclododecane, 1,5-bis[(4-methylphenyl)sulfonyl]-9-(phenylmethyl)- (9CI) (CA INDEX NAME)



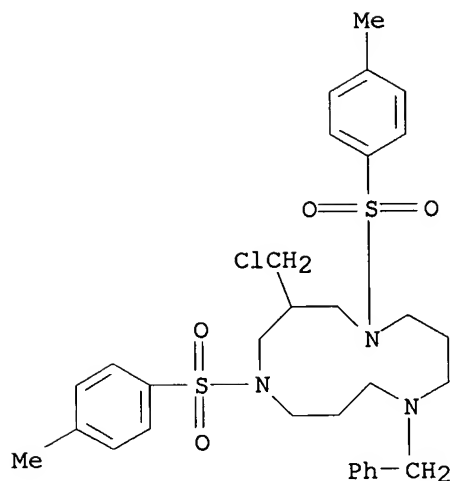
RN 182316-08-1 CAPLUS

CN 1,5,9-Triazacyclododecane-3-methanol, 1,5-bis[(4-methylphenyl)sulfonyl]-9-(phenylmethyl)- (9CI) (CA INDEX NAME)

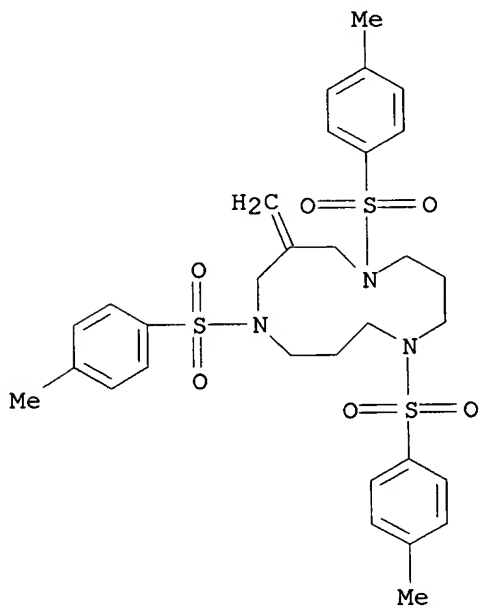


RN 182316-10-5 CAPLUS

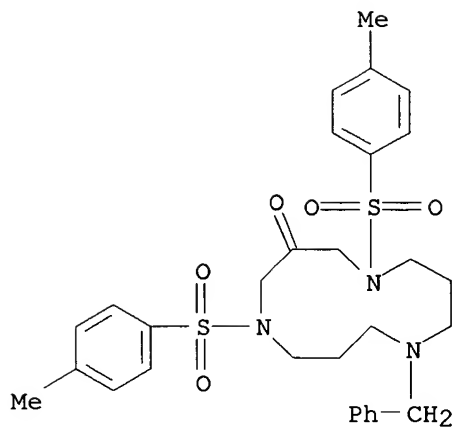
CN 1,5,9-Triazacyclododecane, 3-(chloromethyl)-1,5-bis[(4-methylphenyl)sulfonyl]-9-(phenylmethyl)- (9CI) (CA INDEX NAME)



RN 182316-15-0 CAPLUS
 CN 1,5,9-Triazacyclododecane, 3-methylene-1,5,9-tris[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)

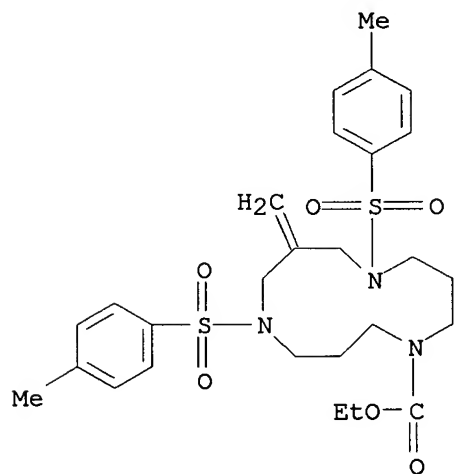


RN 182316-20-7 CAPLUS
 CN 1,5,9-Triazacyclododecan-3-one, 1,5-bis[(4-methylphenyl)sulfonyl]-9-(phenylmethyl)- (9CI) (CA INDEX NAME)



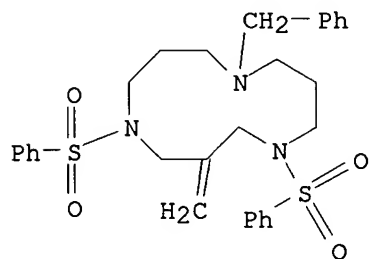
RN 182316-30-9 CAPLUS

CN 1,5,9-Triazacyclododecane-1-carboxylic acid, 7-methylene-5,9-bis[(4-methylphenyl)sulfonyl]-, ethyl ester (9CI) (CA INDEX NAME)



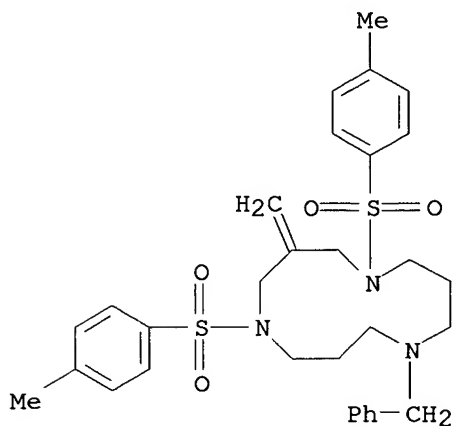
RN 182316-34-3 CAPLUS

CN 1,5,9-Triazacyclododecane, 3-methylene-9-(phenylmethyl)-1,5-bis(phenylsulfonyl)- (9CI) (CA INDEX NAME)



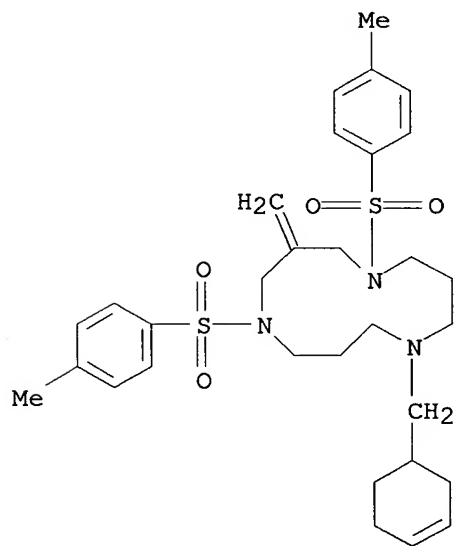
RN 182316-44-5 CAPLUS

CN 1,5,9-Triazacyclododecane, 3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]-9-(phenylmethyl)- (9CI) (CA INDEX NAME)



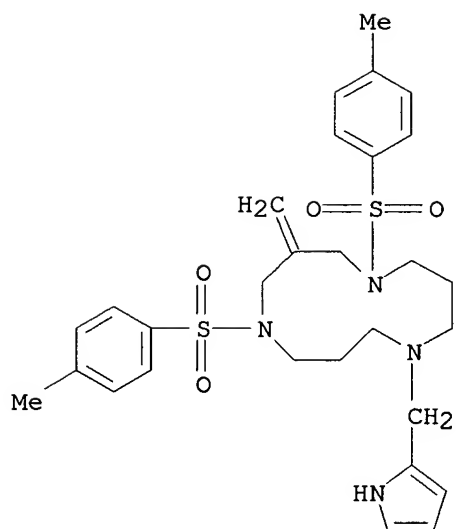
RN 471866-86-1 CAPLUS

CN 1,5,9-Triazacyclododecane, 9-(3-cyclohexen-1-ylmethyl)-3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)



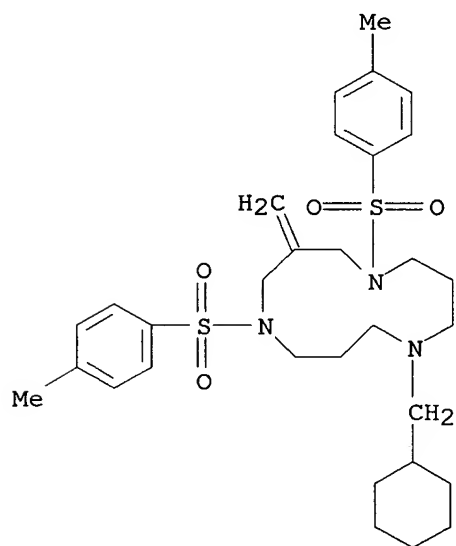
RN 471866-87-2 CAPLUS

CN 1,5,9-Triazacyclododecane, 3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]-9-(1H-pyrrol-2-ylmethyl)- (9CI) (CA INDEX NAME)



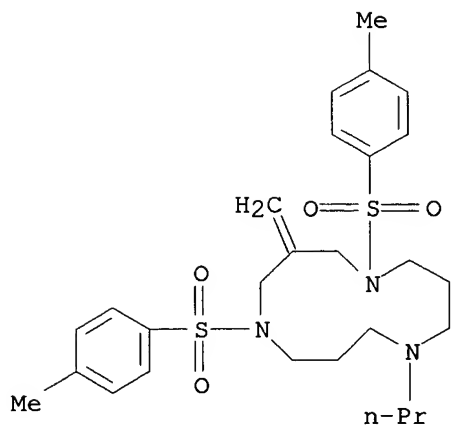
RN 471866-89-4 CAPLUS

CN 1,5,9-Triazacyclododecane, 9-(cyclohexylmethyl)-3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)

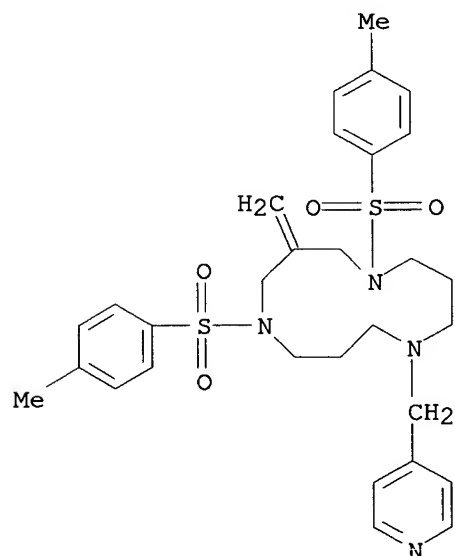


RN 471866-90-7 CAPLUS

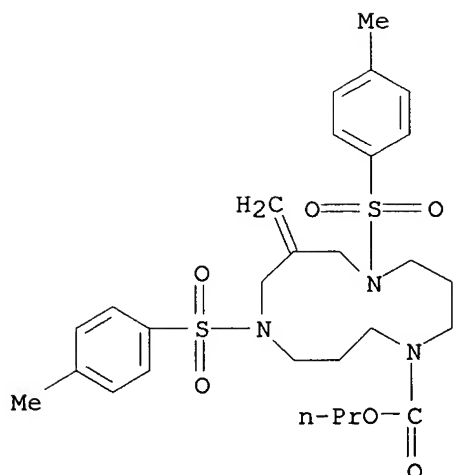
CN 1,5,9-Triazacyclododecane, 3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]-9-propyl- (9CI) (CA INDEX NAME)



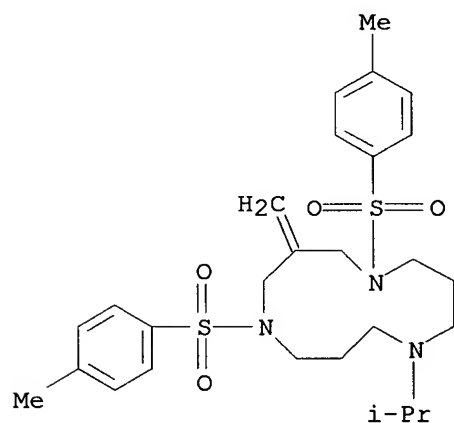
RN 471866-91-8 CAPLUS
 CN 1,5,9-Triazacyclododecane, 3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]-9-(4-pyridinylmethyl)- (9CI) (CA INDEX NAME)



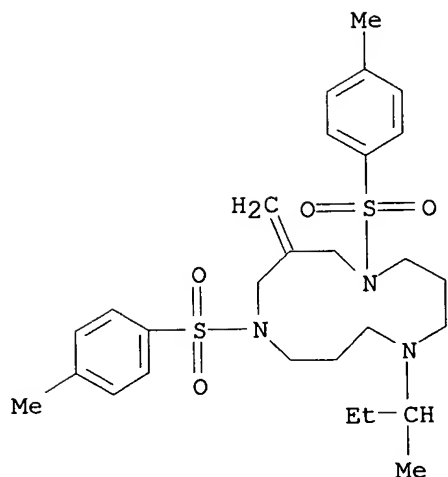
RN 471866-92-9 CAPLUS
 CN 1,5,9-Triazacyclododecane-1-carboxylic acid, 7-methylene-5,9-bis[(4-methylphenyl)sulfonyl]-, propyl ester (9CI) (CA INDEX NAME)



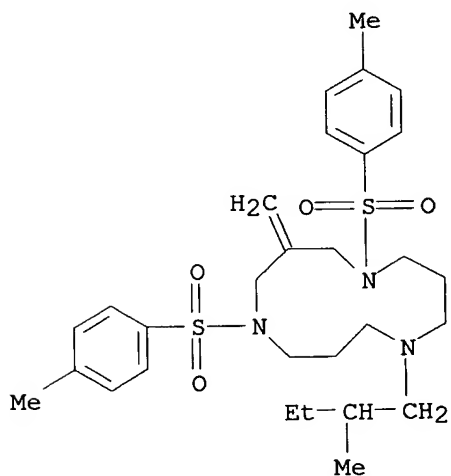
RN 471866-93-0 CAPLUS
 CN 1,5,9-Triazacyclododecane, 3-methylene-9-(1-methylethyl)-1,5-bis[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)



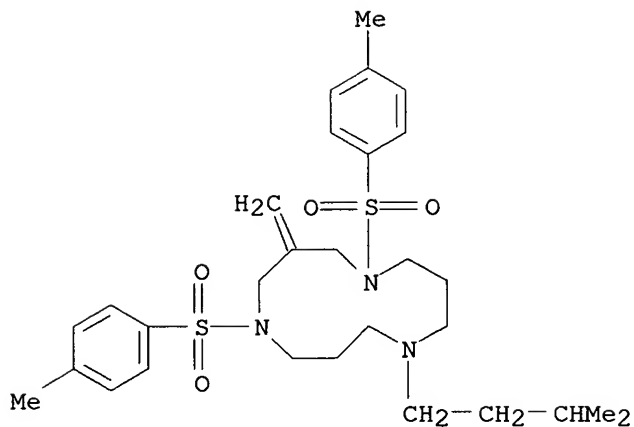
RN 471866-94-1 CAPLUS
 CN 1,5,9-Triazacyclododecane, 3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]-9-(1-methylpropyl)- (9CI) (CA INDEX NAME)



RN 471866-95-2 CAPLUS
 CN 1,5,9-Triazacyclododecane, 9-(2-methylbutyl)-3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)

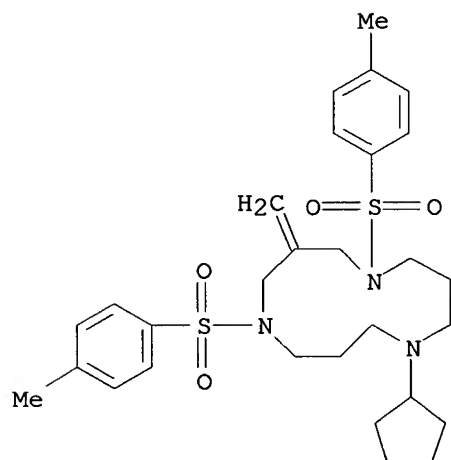


RN 471866-96-3 CAPLUS
 CN 1,5,9-Triazacyclododecane, 9-(3-methylbutyl)-3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)



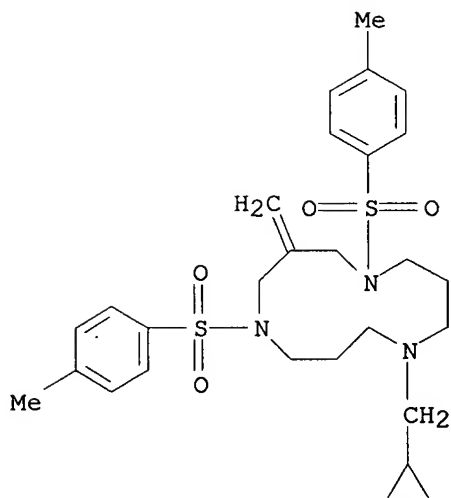
RN 471866-97-4 CAPLUS

CN 1,5,9-Triazacyclododecane, 9-cyclopentyl-3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)



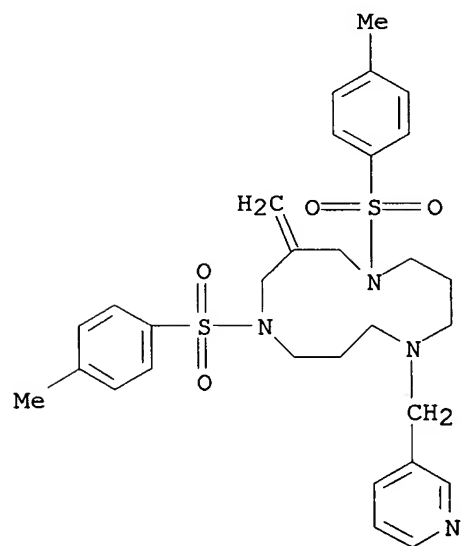
RN 471866-98-5 CAPLUS

CN 1,5,9-Triazacyclododecane, 9-(cyclopropylmethyl)-3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)



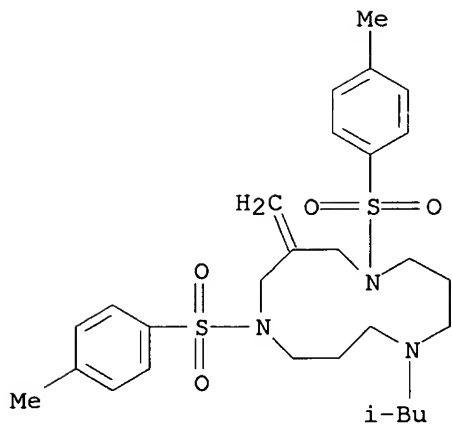
RN 471866-99-6 CAPLUS

CN 1,5,9-Triazacyclododecane, 3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]-9-(3-pyridinylmethyl)- (9CI) (CA INDEX NAME)



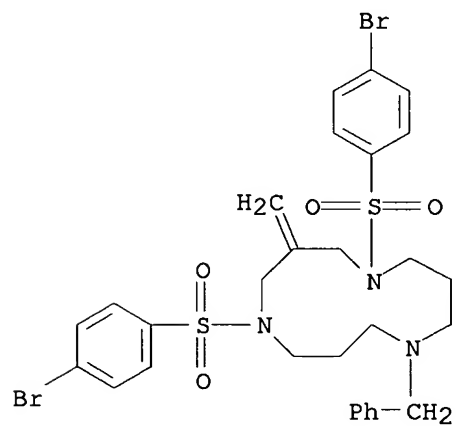
RN 471867-00-2 CAPLUS

CN 1,5,9-Triazacyclododecane, 3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]-9-(2-methylpropyl)- (9CI) (CA INDEX NAME)



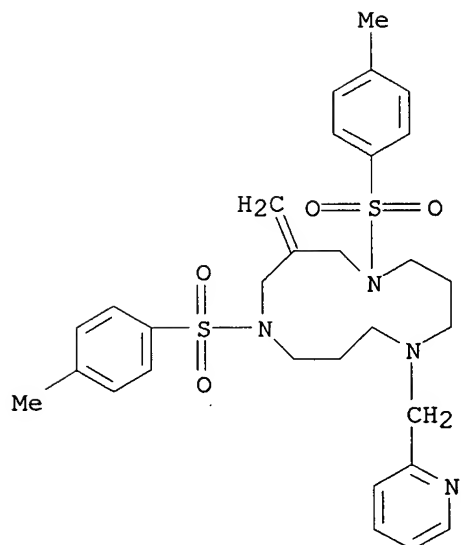
RN 471867-02-4 CAPLUS

CN 1,5,9-Triazacyclododecane, 1,5-bis[(4-bromophenyl)sulfonyl]-3-methylene-9-(phenylmethyl)- (9CI) (CA INDEX NAME)



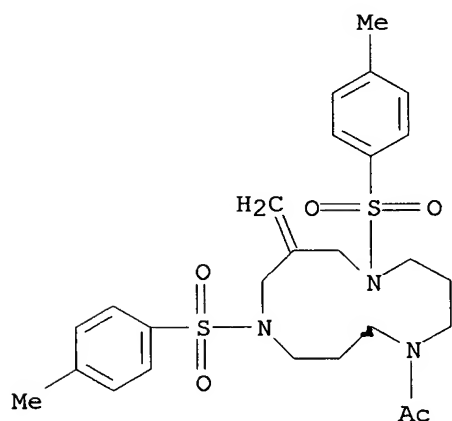
RN 471867-03-5 CAPLUS

CN 1,5,9-Triazacyclododecane, 3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]-9-(2-pyridinylmethyl)- (9CI) (CA INDEX NAME)



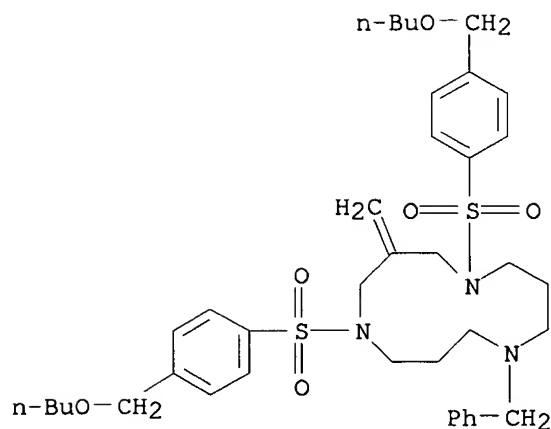
RN 471867-04-6 CAPLUS

CN 1,5,9-Triazacyclododecane, 9-acetyl-3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)



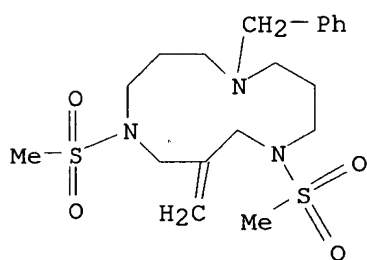
RN 471867-05-7 CAPLUS

CN 1,5,9-Triazacyclododecane, 1,5-bis[[4-(butoxymethyl)phenyl]sulfonyl]-3-methylene-9-(phenylmethyl)- (9CI) (CA INDEX NAME)



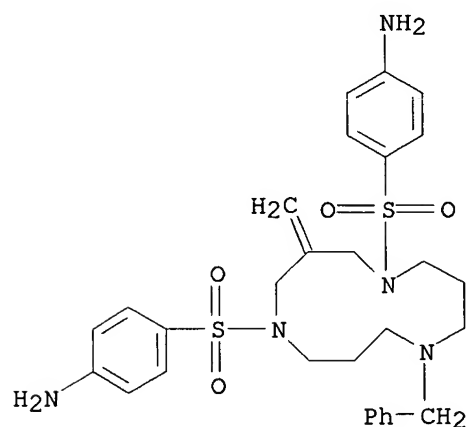
RN 471867-06-8 CAPLUS

CN 1,5,9-Triazacyclododecane, 3-methylene-1,5-bis(methylsulfonyl)-9-(phenylmethyl)- (9CI) (CA INDEX NAME)



RN 544430-76-4 CAPLUS

CN 1,5,9-Triazacyclododecane, 1,5-bis[(4-aminophenyl)sulfonyl]-3-methylene-9-(phenylmethyl)- (9CI) (CA INDEX NAME)



REFERENCE COUNT:

27

THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

10/680,076

~~130~~ ANSWER 12 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2002:880548 CAPLUS

DOCUMENT NUMBER: 138:140271

TITLE: Strongly basic macrocyclic triamines,
1,5,9-triazacyclododecanes for solvent extraction of
gold(I) cyanide

AUTHOR(S): Choi, Heung-Jin; Bae, Yoon-Kyung; Kang, Seok-Chan;
Park, Yeon Sil; Park, Joon Won; Kim, Woong-Il; Bell,
Thomas W.

CORPORATE SOURCE: Department of Industrial Chemistry, Kyungpook National
University, Taegu, 702-701, S. Korea

SOURCE: Tetrahedron Letters (2002), 43(51), 9385-9389

CODEN: TELEAY; ISSN: ~~0040-4039~~

PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Solvent extraction of gold(I) dicyanide anion from alkaline gold(I) cyanide
solution

by using unusually basic amine extractants was conducted. The
1,5,9-Triazacyclododecane (IV) is known as an unusually basic macrocyclic
amine having $pK_a = 12.3-12.7$ and is thus a candidate as a basic amine
extractant. Three lipophilic derivs. of IV expected to stay in the organic
phase during gold solvent extraction were synthesized. N-Dodecyl-1,5,9-
triazacyclododecane (III) was prepared from 1,5,9-triazacyclododecane-2,4-
dione (I) by N-alkylation with n-dodecyl iodide and then reduction with
BH₃-THF. N,N'-Didodecyl-1,5,9-triazacyclododecane (V) and
N,N',N''-tridodecyl-1,5,9-triazacyclododecane (VI) were efficiently
synthesized by selective di-alkylation of IV with n-dodecyl iodide, and by
reductive alkylation of IV with n-dodecanol, resp. Extractants III and VI
extracted 50% of the metal at pH 10.5, which is the min. value required for
practical application.

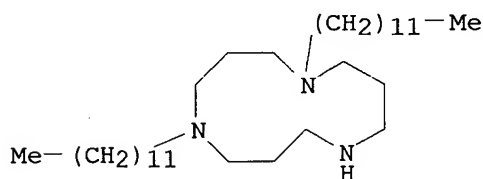
IT 494769-64-1 494769-65-2

RL: PEP (Physical, engineering or chemical process); PYP (Physical
process); PROC (Process)

(strongly basic macrocyclic triamines as extractants for solvent extraction
of gold(I) cyanide)

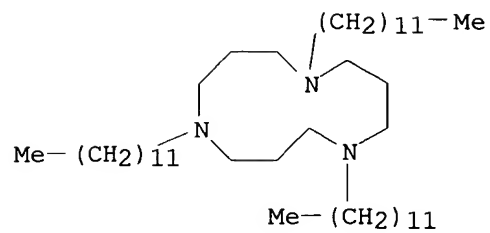
RN 494769-64-1 CAPLUS

CN 1,5,9-Triazacyclododecane, 1,5-didodecyl- (9CI) (CA INDEX NAME)



RN 494769-65-2 CAPLUS

CN 1,5,9-Triazacyclododecane, 1,5,9-tridodecyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT:

26

THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

~~130~~ ANSWER 13 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2002:851418 CAPLUS

DOCUMENT NUMBER: 138:395471

TITLE: CADA Inhibits Human Immunodeficiency Virus and Human Herpesvirus 7 Replication by Down-modulation of the Cellular CD4 Receptor

AUTHOR(S): Vermeire, Kurt; Zhang, Ying; Princen, Katrien; Hatse, Sigrid; Samala, Meinrado F.; Dey, Kaka; Choi, Heung-Jin; Ahn, Youngmi; Sodoma, Andrej; Snoeck, Robert; Andrei, Graciela; De Clercq, Erik; Bell, Thomas W.; Schols, Dominique

CORPORATE SOURCE: Rega Institute for Medical Research, Katholieke Universiteit Leuven, Louvain, B-3000, Belg.

SOURCE: Virology (2002), 302(2), 342-353

CODEN: VIRLAX; ISSN: 0042-6822

PUBLISHER: Elsevier Science

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The novel antiviral agent cyclootriazadisulfonamide (CADA) inhibited human immunodeficiency virus (HIV) (IC₅₀, 0.3-3.2 μ M) and human herpesvirus 7 (HHV-7) infection (IC₅₀, 0.3-1.5 μ M) in T-cell lines and PBMCs. When T-cells were pretreated with CADA for 24 h, they became markedly protected from viral infection. Flow cytometric anal. revealed a significant decrease in the expression of the CD4 glycoprotein, the primary receptor needed for entry of both viruses. Moreover, the antiviral activity of CADA correlated with its ability to down-modulate the CD4 receptor. CADA did not alter the expression of any other cellular receptor (or HIV coreceptor) examined. Time course expts. showed that CD4 down-modulation by CADA differs in mechanism from the effects of aurintricarboxylic acid, which binds directly to CD4, and phorbol myristate acetate, which activates protein kinase C. Further anal. of CD4 mRNA levels suggested that CADA was not involved in the regulation of CD4 expression at a transcriptional level, but very likely at (post) translational levels. This unique mechanism of action makes CADA an important lead in developing new drugs for treatment of AIDS, autoimmune diseases, and inflammatory disorders.

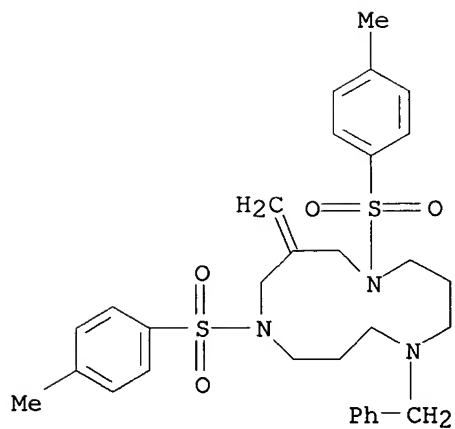
IT 392287-03-5

RL: DMA (Drug mechanism of action); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(cyclootriazadisulfonamide (CADA) inhibits human immunodeficiency virus and human herpesvirus 7 replication by down-modulation of cellular CD4 receptor)

RN 392287-03-5 CAPLUS

CN 1,5,9-Triazacyclododecane, 3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]-9-(phenylmethyl)-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

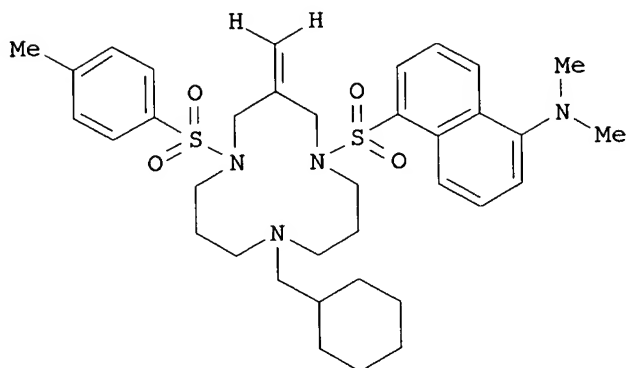
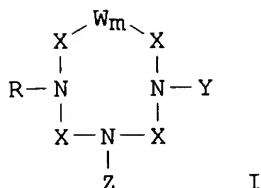
REFERENCE COUNT:

47

THERE ARE 47 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L30 ANSWER 14 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN
 ACCESSION NUMBER: 2002:793364 CAPLUS
 DOCUMENT NUMBER: 137:304743
 TITLE: Macrocyclic triaza compounds as immunoregulatory agents
 INVENTOR(S): Bell, Thomas W.; Schols, Dominique; Dey, Kaka; Vermeire, Kurt
 PATENT ASSIGNEE(S): University and Community College System of Nevada on Behalf of the University of Nevada, Reno, USA
 SOURCE: PCT Int. Appl., 70 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002080856	A2	20021017	WO 2002-US11223	20020408
WO 2002080856	A3	20040318		
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW			
RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
AU 2002303293	A1	20021021	AU 2002-303293	20020408
US 2004220164	A1	20041104	US 2003-680076	20031006
PRIORITY APPLN. INFO.:			US 2001-282212P	P 20010406
			WO 2002-US11223	W 20020408
OTHER SOURCE(S):	MARPAT 137:304743			
GI				



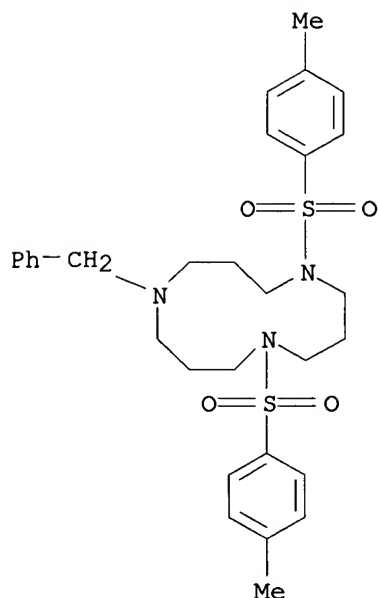
AB Title compds. I [W = a bridge carbon which is unsubstituted or is bonded directly or indirectly to one or two polar or non-polar side group substituents; R and Y independently = (un)substituted aryl, alkyl or alkenyl attached through an optional linker group; Z = H, (un)substituted aryl, alkyl or alkenyl attached through a linking group; X = Ca-d which represents carbon bridges, preferably alkylene bridges, between nitrogens, the length of which is defined by the subscripts a-d, the bridges may be optionally substituted and saturated or unsatd.; a and d independently = 0-10; b and c independently = 1-10; m = 0-3], which down-regulate CD4 expression for use in the treatment of autoimmune diseases and inflammatory diseases or conditions, are disclosed. In a specific embodiment, the invention provides certain naphthalene substituted triaza macrocycles which exhibit high activity for down regulation of CD4 expression. In particular, triaza macrocycles having dansyl groups, e.g., II, are provided for use in pharmaceutical compns. II possessed an IC50 ($\mu\text{g/mL}$) value of 0.41 in assays to determine CD4 down-modulating activity in MT-4 cells.

IT 164913-15-9 182316-08-1 182316-10-5
 182316-15-0 182316-20-7 182316-30-9
 182316-44-5 392287-03-5 471866-86-1
 471866-87-2 471866-89-4 471866-90-7
 471866-91-8 471866-92-9 471866-93-0
 471866-94-1 471866-95-2 471866-96-3
 471866-97-4 471866-98-5 471866-99-6
 471867-00-2 471867-01-3 471867-02-4
 471867-03-5 471867-04-6 471867-05-7
 471867-06-8

RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
 (Biological study); USES (Uses)
 (evaluation of triazamacrocycles as immunoregulatory agents with CD4
 down-modulating activity)

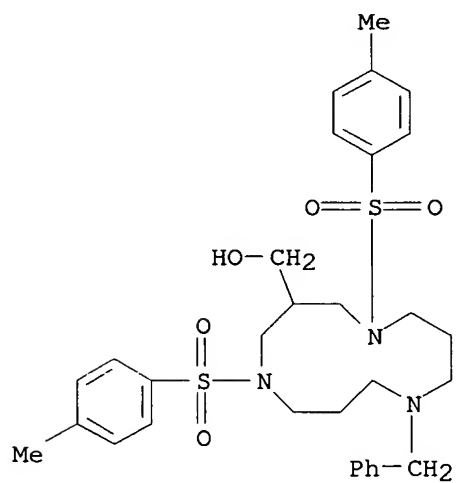
RN 164913-15-9 CAPLUS

CN 1,5,9-Triazacyclododecane, 1,5-bis[(4-methylphenyl)sulfonyl]-9-
 (phenylmethyl)- (9CI) (CA INDEX NAME)



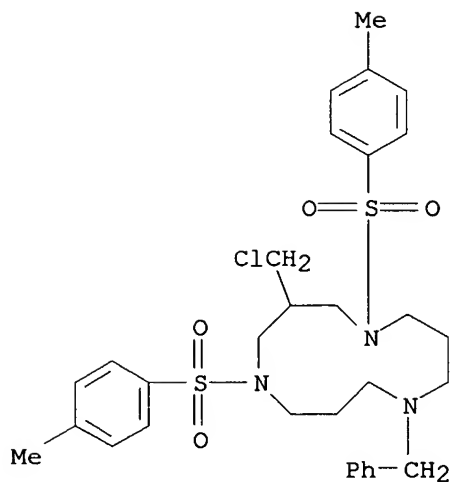
RN 182316-08-1 CAPLUS

CN 1,5,9-Triazacyclododecane-3-methanol, 1,5-bis[(4-methylphenyl)sulfonyl]-9-(phenylmethyl)- (9CI) (CA INDEX NAME)



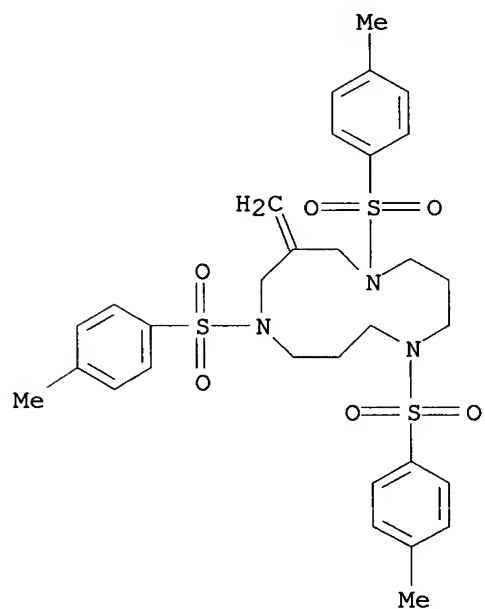
RN 182316-10-5 CAPLUS

CN 1,5,9-Triazacyclododecane, 3-(chloromethyl)-1,5-bis[(4-methylphenyl)sulfonyl]-9-(phenylmethyl)- (9CI) (CA INDEX NAME)



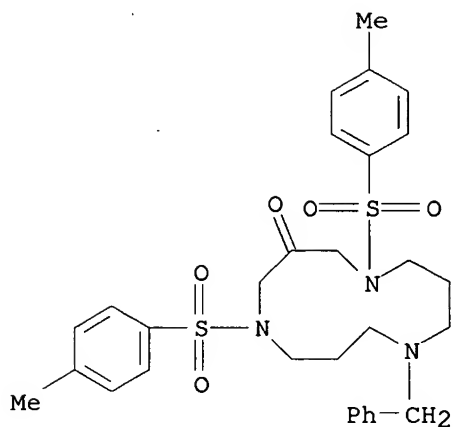
RN 182316-15-0 CAPLUS

CN 1,5,9-Triazacyclododecane, 3-methylene-1,5,9-tris[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)

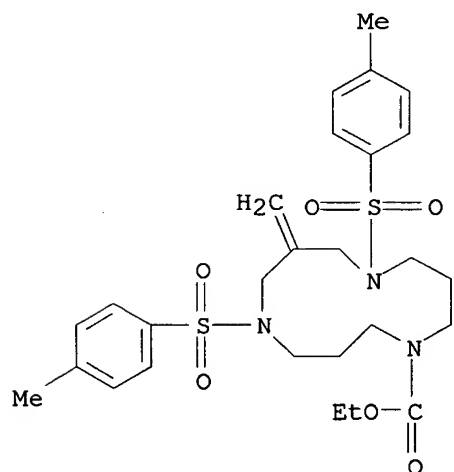


RN 182316-20-7 CAPLUS

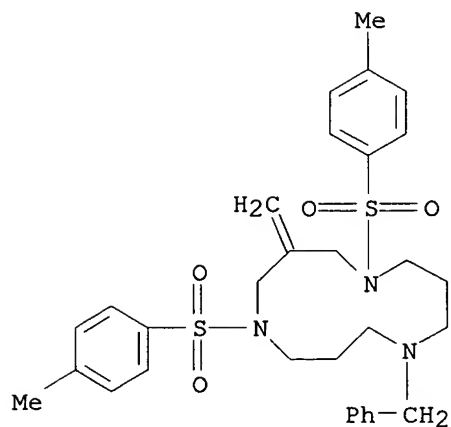
CN 1,5,9-Triazacyclododecan-3-one, 1,5-bis[(4-methylphenyl)sulfonyl]-9-(phenylmethyl)- (9CI) (CA INDEX NAME)



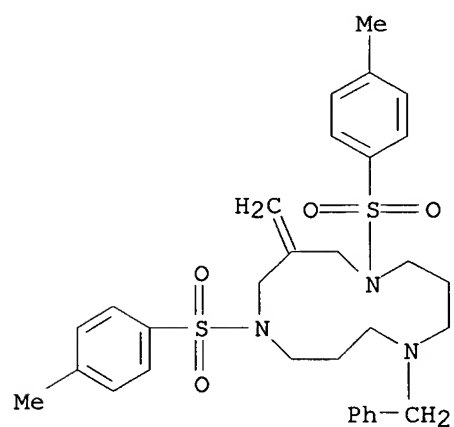
RN 182316-30-9 CAPLUS
 CN 1,5,9-Triazacyclododecane-1-carboxylic acid, 7-methylene-5,9-bis[(4-methylphenyl)sulfonyl]-, ethyl ester (9CI) (CA INDEX NAME)



RN 182316-44-5 CAPLUS
 CN 1,5,9-Triazacyclododecane, 3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]-9-(phenylmethyl)- (9CI) (CA INDEX NAME)

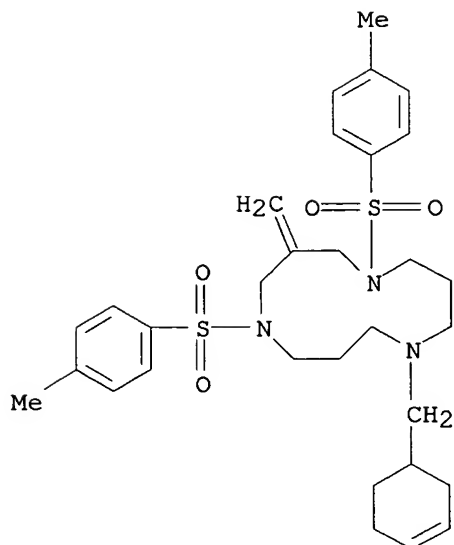


RN 392287-03-5 CAPLUS
 CN 1,5,9-Triazacyclododecane, 3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]-9-(phenylmethyl)-, monohydrochloride (9CI) (CA INDEX NAME)



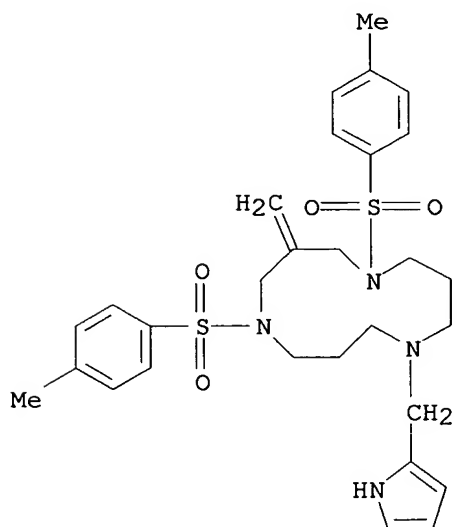
● HCl

RN 471866-86-1 CAPLUS
 CN 1,5,9-Triazacyclododecane, 9-(3-cyclohexen-1-ylmethyl)-3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)



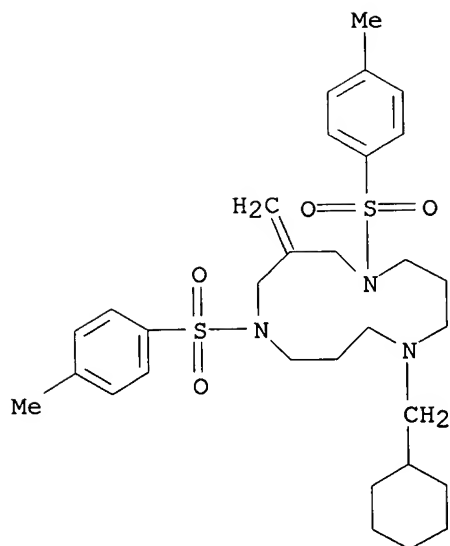
RN 471866-87-2 CAPLUS

CN 1,5,9-Triazacyclododecane, 3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]-9-(1H-pyrrol-2-ylmethyl)- (9CI) (CA INDEX NAME)

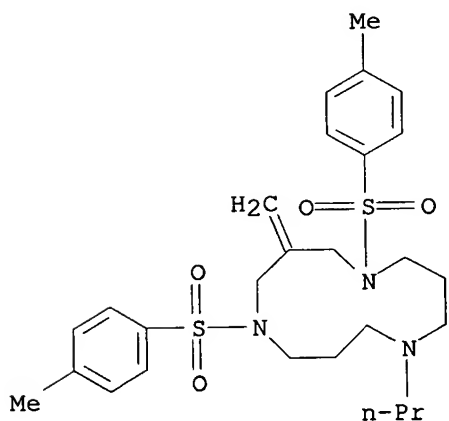


RN 471866-89-4 CAPLUS

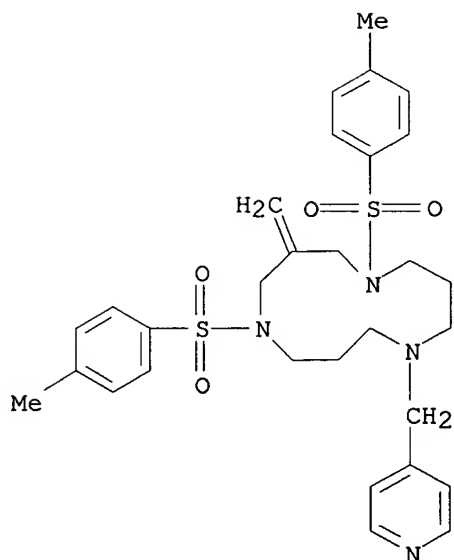
CN 1,5,9-Triazacyclododecane, 9-(cyclohexylmethyl)-3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)



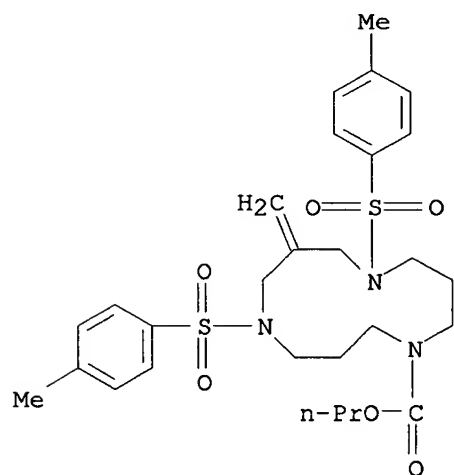
RN 471866-90-7 CAPLUS
 CN 1,5,9-Triazacyclododecane, 3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]-9-propyl- (9CI) (CA INDEX NAME)



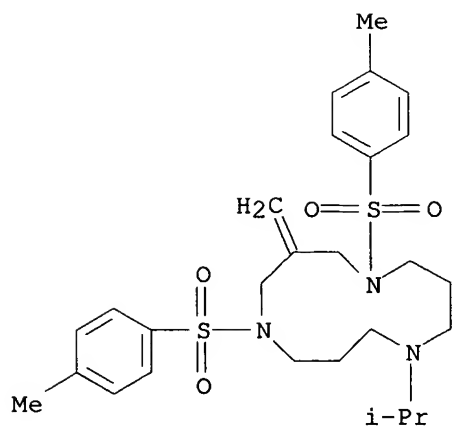
RN 471866-91-8 CAPLUS
 CN 1,5,9-Triazacyclododecane, 3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]-9-(4-pyridinylmethyl)- (9CI) (CA INDEX NAME)



RN 471866-92-9 CAPLUS
 CN 1,5,9-Triazacyclododecane-1-carboxylic acid, 7-methylene-5,9-bis[(4-methylphenyl)sulfonyl]-, propyl ester (9CI) (CA INDEX NAME)

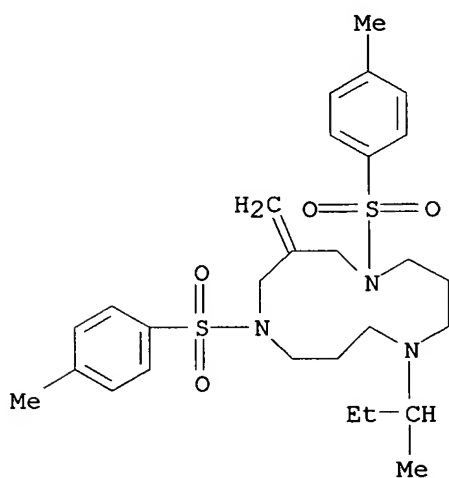


RN 471866-93-0 CAPLUS
 CN 1,5,9-Triazacyclododecane, 3-methylene-9-(1-methylethyl)-1,5-bis[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)



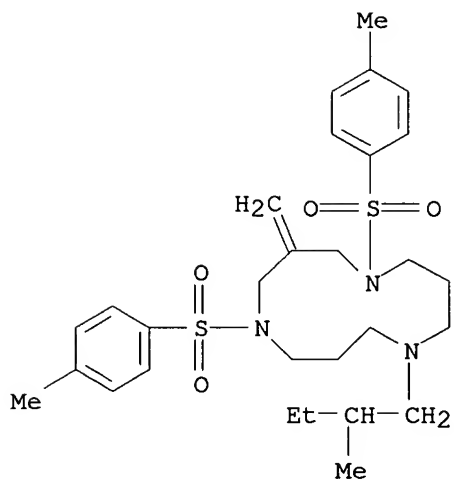
RN 471866-94-1 CAPLUS

CN 1,5,9-Triazacyclododecane, 3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]-9-(1-methylpropyl)- (9CI) (CA INDEX NAME)



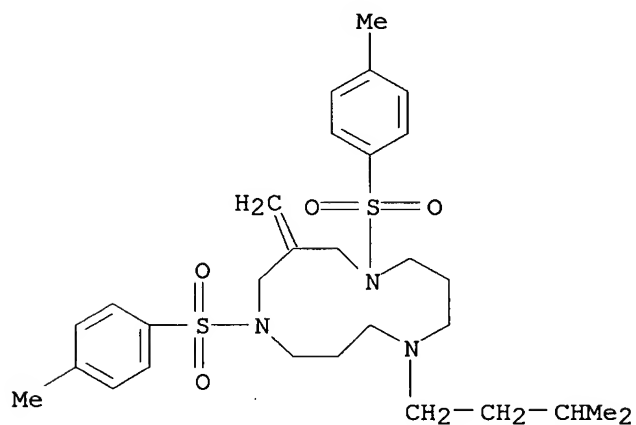
RN 471866-95-2 CAPLUS

CN 1,5,9-Triazacyclododecane, 9-(2-methylbutyl)-3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)



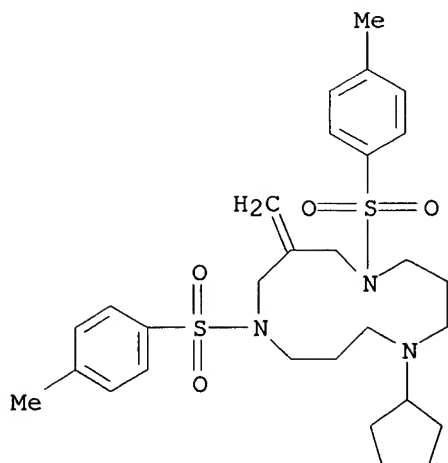
RN 471866-96-3 CAPLUS

CN 1,5,9-Triazacyclododecane, 9-(3-methylbutyl)-3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)



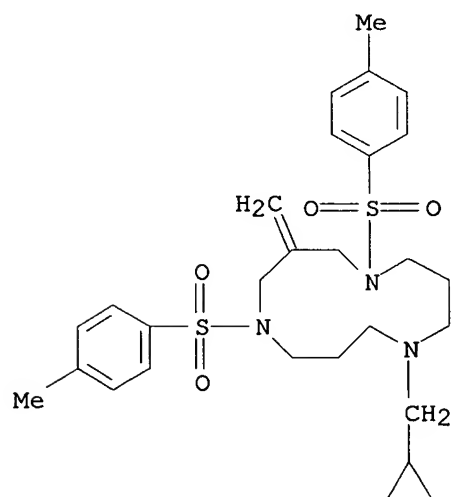
RN 471866-97-4 CAPLUS

CN 1,5,9-Triazacyclododecane, 9-cyclopentyl-3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)



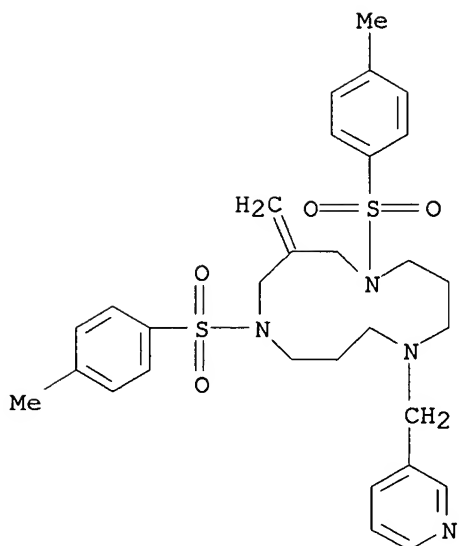
RN 471866-98-5 CAPLUS

CN 1,5,9-Triazacyclododecane, 9-(cyclopropylmethyl)-3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)



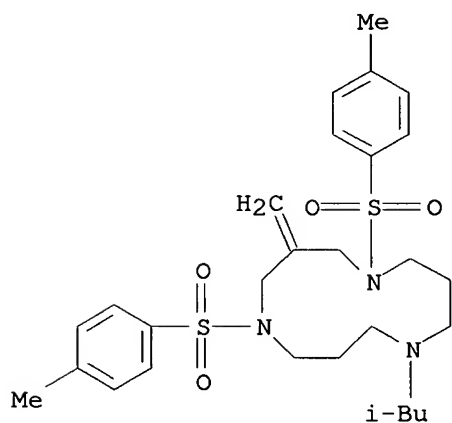
RN 471866-99-6 CAPLUS

CN 1,5,9-Triazacyclododecane, 3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]-9-(3-pyridinylmethyl)- (9CI) (CA INDEX NAME)



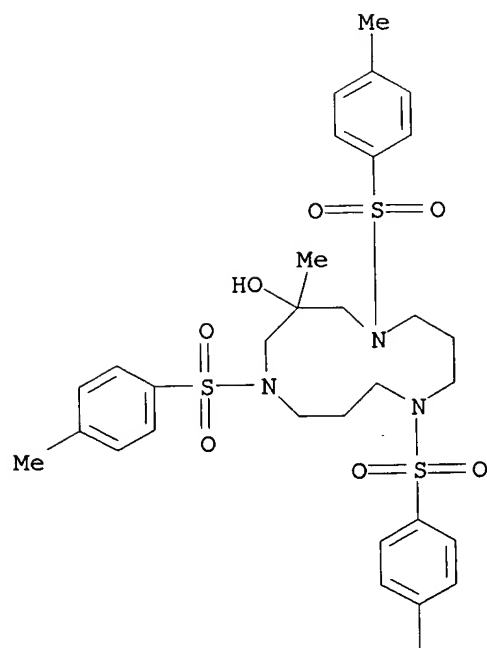
RN 471867-00-2 CAPLUS

CN 1,5,9-Triazacyclododecane, 3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]-9-(2-methylpropyl)- (9CI) (CA INDEX NAME)

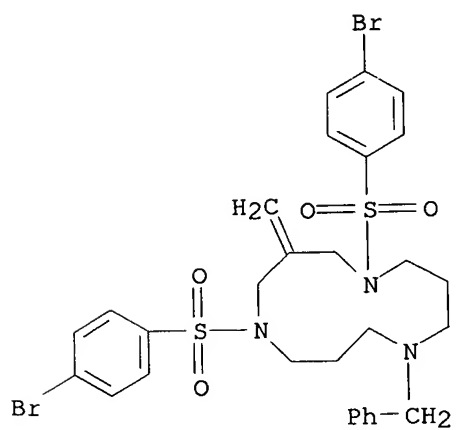


RN 471867-01-3 CAPLUS

CN 1,5,9-Triazacyclododecan-3-ol, 3-methyl-1,5,9-tris[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)

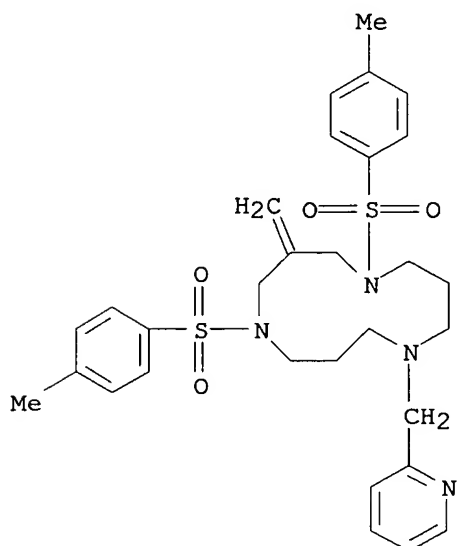


RN 471867-02-4 CAPLUS
 CN 1,5,9-Triazacyclododecane, 1,5-bis[(4-bromophenyl)sulfonyl]-3-methylene-9-(phenylmethyl)- (9CI) (CA INDEX NAME)



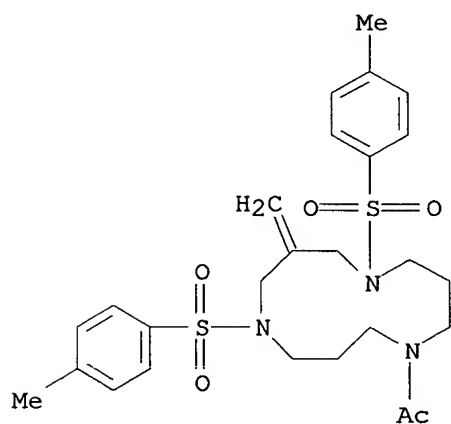
RN 471867-03-5 CAPLUS

CN 1,5,9-Triazacyclododecane, 3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]-9-(2-pyridinylmethyl)- (9CI) (CA INDEX NAME)



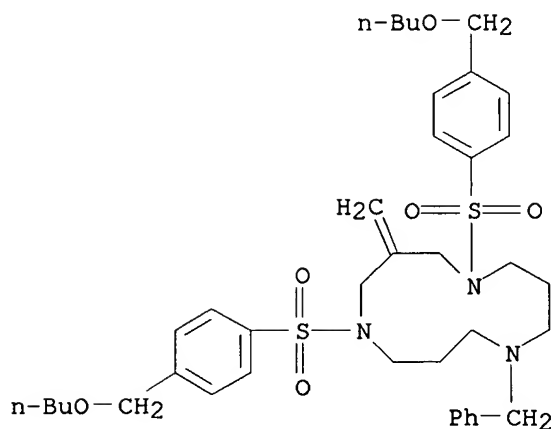
RN 471867-04-6 CAPLUS

CN 1,5,9-Triazacyclododecane, 9-acetyl-3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)



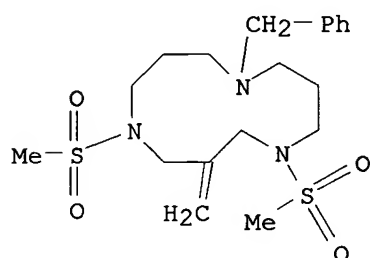
RN 471867-05-7 CAPLUS

CN 1,5,9-Triazacyclododecane, 1,5-bis[[4-(butoxymethyl)phenyl]sulfonyl]-3-methylene-9-(phenylmethyl)- (9CI) (CA INDEX NAME)



RN 471867-06-8 CAPLUS

CN 1,5,9-Triazacyclododecane, 3-methylene-1,5-bis(methylsulfonyl)-9-(phenylmethyl)- (9CI) (CA INDEX NAME)



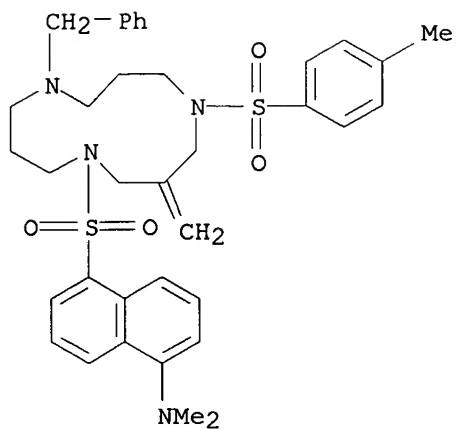
IT 471866-79-2P 471866-80-5P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation and biol. activity of naphthalenesulfonyl triazamacrocycles as immunoregulatory agents)

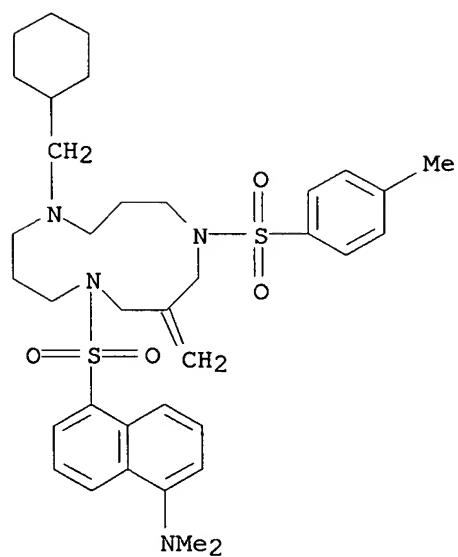
RN 471866-79-2 CAPLUS

CN 1,5,9-Triazacyclododecane, 1-[[5-(dimethylamino)-1-naphthalenyl]sulfonyl]-3-methylene-5-[(4-methylphenyl)sulfonyl]-9-(phenylmethyl)- (9CI) (CA INDEX NAME)



RN 471866-80-5 CAPLUS

CN 1,5,9-Triazacyclododecane, 9-(cyclohexylmethyl)-1-[[5-(dimethylamino)-1-naphthalenyl]sulfonyl]-3-methylene-5-[(4-methylphenyl)sulfonyl]- (9CI)
(CA INDEX NAME)



190 ANSWER 15 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2002:359518 CAPLUS

DOCUMENT NUMBER: 137:194461

TITLE: Synthesis, characterisation and polymerization of vinylbenzene-substituted triazacyclododecanes and their transition metal complexes

AUTHOR(S): Long, Nicholas J.; Parker, David G.; Speyer, Paul R.; White, Andrew J. P.; Williams, David J.

CORPORATE SOURCE: Department of Chemistry, Imperial College of Science, Technology and Medicine, South Kensington, London, SW7 2AY, UK

SOURCE: Journal of the Chemical Society, Dalton Transactions (2002), (10), 2142-2150

CODEN: JCSDAA; ISSN: 1472-7773

PUBLISHER: Royal Society of Chemistry

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 137:194461

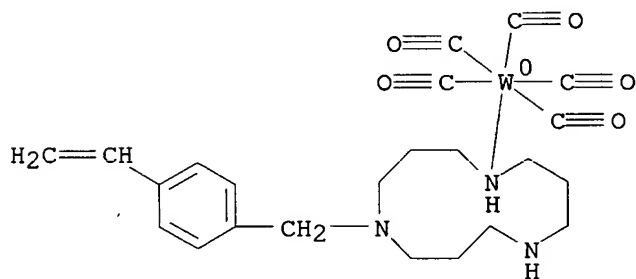
AB The synthesis of a range of methylated and nonmethylated triazacyclododecane derivs. featuring the unsym. incorporation of a 4-vinylbenzene side-arm is reported, along with the x-ray crystal structure of an amidinium salt precursor, and NMR characterization of these ligands. The free amine, 1-(4-vinylbenzyl)-1,5,9-triazacyclododecane (5), was reacted with transition metal centers and the coordination chemical is discussed, with structural anal. of an unusual triply-bridged (via one aqua and two chloride ligands) Ni(II) dimer and a mononuclear W(CO)₅ complex. Co-polymerization studies on 5 and its metal complexes with varying percentages of styrene show the formation of low and high (via crosslinking) mol. weight polymers.

IT 448898-76-8P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (preparation and crystal structure)

RN 448898-76-8 CAPLUS

CN Tungsten, pentacarbonyl[1-[(4-ethenylphenyl)methyl]-1,5,9-triazacyclododecane-κN5]-, (OC-6-22)- (9CI) (CA INDEX NAME)

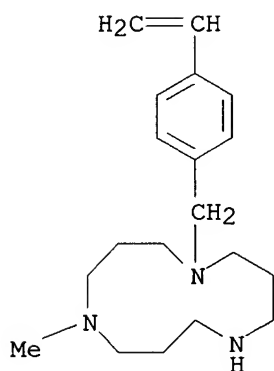


IT 243670-33-9P, 1-Methyl-5-(4-vinylbenzyl)-1,5,9-triazacyclododecane

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation and methylation)

RN 243670-33-9 CAPLUS

CN 1,5,9-Triazacyclododecane, 1-[(4-ethenylphenyl)methyl]-5-methyl- (9CI) (CA INDEX NAME)

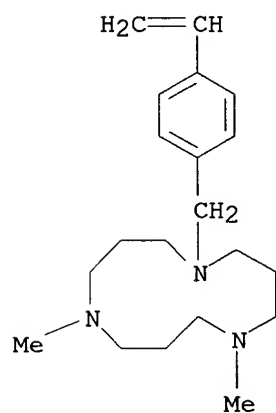


IT 243670-34-0P, 5,9-Dimethyl-1-(4-vinylbenzyl)-1,5,9-triazacyclododecane

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 243670-34-0 CAPLUS

CN 1,5,9-Triazacyclododecane, 1-[(4-ethenylphenyl)methyl]-5,9-dimethyl- (9CI)
(CA INDEX NAME)



REFERENCE COUNT:

51

THERE ARE 51 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

100 ANSWER 16 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2002:271332 CAPLUS

DOCUMENT NUMBER: 137:118540

TITLE: Synthesis and characterization of the zinc(II)-fluorophore, 5-dimethylaminonaphthalene-1-sulfonic acid [2-(1,5,9-triazacyclododec-1-yl)ethyl]amide and its zinc(II) complex
 AUTHOR(S): Koike, Tohru; Abe, Tomoko; Takahashi, Makoto; Ohtani, Kazuhiro; Kimura, Eiichi; Shiro, Motoo
 CORPORATE SOURCE: Institute of Pharmaceutical Sciences, Faculty of Medicine, Hiroshima University, Minami-ku, Hiroshima, Japan

SOURCE: Journal of the Chemical Society, Dalton Transactions (2002), (8), 1764-1768

(CODEN: JCSDAA; ISSN: 1472-7773

PUBLISHER: Royal Society of Chemistry

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 137:118540

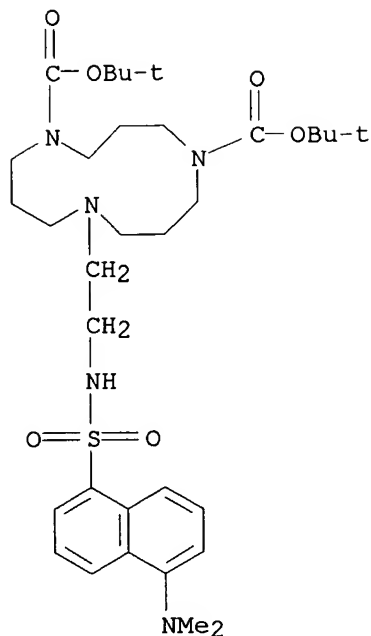
AB A new Zn(II)-fluorophore, 5-dimethylaminonaphthalene-1-sulfonic acid [2-(1,5,9-triazacyclododec-1-yl)ethyl]amide (HL) was synthesized and characterized. The spectrophotometric and potentiometric pH-titration study disclosed a 1:1 Zn(II) complexation with a stability constant, $K(\text{ZnL})$ of 101.3 ($= [\text{ZnL}]/[\text{Zn}^{2+}][\text{HL}]$) at 25° with $I = 0.10$ (NaCl) in aqueous solution, where L is the dansylamide deprotonated ligand. The fluorescence intensity of ZnL at 538 nm (excitation at 320 nm) is 5.2 times greater than that of the ligand (HL·H⁺ form) in aqueous solution at pH 7.8 and 25° with $I = 0.10$ (NaCl). The x-ray crystal anal. of the Zn(II) complex $[\text{ZnL}(\text{ClO}_4) \cdot \text{EtOH}]$ showed a four-coordinate Zn(II) with three N atoms of the macrocyclic triamine and the dansylamide N⁻ anion.

IT 443643-93-4P

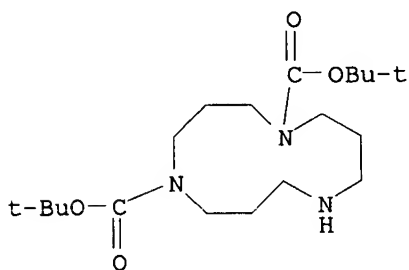
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation and deprotection of)

RN 443643-93-4 CAPLUS

CN 1,5,9-Triazacyclododecane-1,5-dicarboxylic acid, 9-[2-[[[5-(dimethylamino)-1-naphthalenyl]sulfonyl]amino]ethyl]-, bis(1,1-dimethylethyl) ester (9CI)
 (CA INDEX NAME)



IT 174192-40-6, 1,5-Bis(tert-butoxycarbonyl)-1,5,9-triazacyclododecane
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (reactant for preparation of aminonaphthalenesulfonyltriazacyclododecylethyl amide)
 RN 174192-40-6 CAPLUS
 CN 1,5,9-Triazacyclododecane-1,5-dicarboxylic acid, bis(1,1-dimethylethyl) ester (9CI) (CA INDEX NAME)

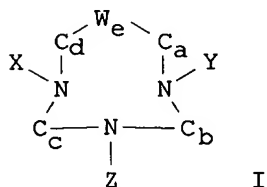


REFERENCE COUNT: 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L30 ANSWER 17 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN

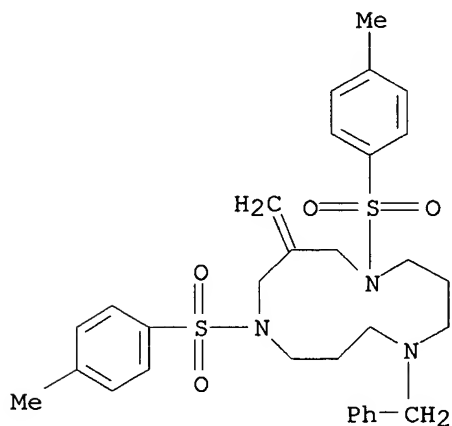
ACCESSION NUMBER: 2002:84595 CAPLUS
 DOCUMENT NUMBER: 136:129039
 TITLE: Antiviral triaza compounds and compositions, and preparation thereof
 INVENTOR(S): Bell, Thomas W.
 PATENT ASSIGNEE(S): The Research Foundation of State University of New York, USA
 SOURCE: U.S., 19 pp., Cont.-in-part of U.S. 5,663,161.
 CODEN: USXXAM
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 2
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 6342492	B1	20020129	US 1997-894491	19970807
US 5663161	A	19970902	US 1995-392550	19950217
WO 9625167	A1	19960822	WO 1996-US2132	19960216
W: AM, AT, AU, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LT, LU, LV, MD, MG, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, TJ, TM, TT RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
US 2002019423	A1	20020214	US 2001-769021	20010125
PRIORITY APPLN. INFO.:			US 1995-392550	A2 19950217
			WO 1996-US2132	W 19960216
			US 1997-894491	A1 19970807
OTHER SOURCE(S):		MARPAT 136:129039		
GI				



AB Synthetic triaza compds. I (W = bridge carbon with polar or nonpolar side group; X, Y = aromatic group, alkyl group, sulfonyl group, , carbonyl group; Z = X, Y, H, fused aryl; a, d, e = 0-10, b, c = 1-10) are disclosed which can be used in antiviral pharmaceutical compns. Preparation of e.g. 9-benzyl-3-methylene-1,5-ditosyl-1,5,9-triazacyclododecane is described. Synthesis of open-chain analogs is also described.
 IT 182316-44-5P
 RL: DMA (Drug mechanism of action); PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
 (antiviral triaza compds., compns., and preparation)
 RN 182316-44-5 CAPLUS

CN 1,5,9-Triazacyclododecane, 3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]-9-(phenylmethyl)- (9CI) (CA INDEX NAME)

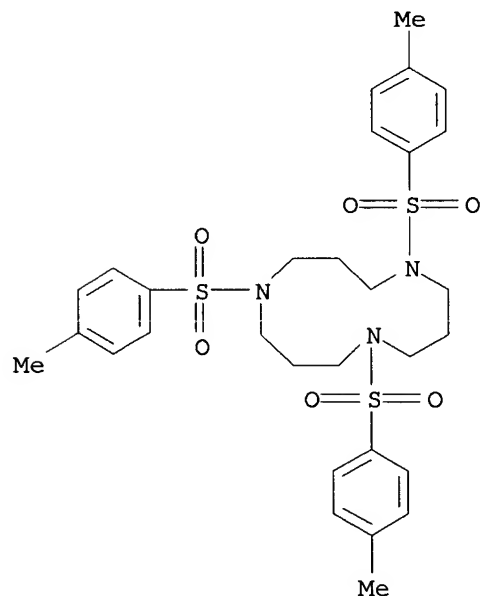


IT 35980-67-7P

RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(antiviral triaza compds., compns., and preparation)

RN 35980-67-7 CAPLUS

CN 1,5,9-Triazacyclododecane, 1,5,9-tris[(4-methylphenyl)sulfonyl]- (9CI)
(CA INDEX NAME)



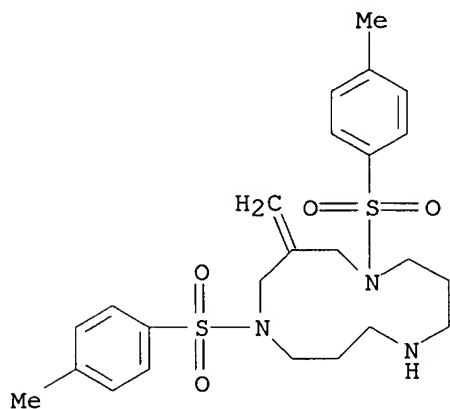
IT 182316-06-9 182316-17-2

RL: PAC (Pharmacological activity); RCT (Reactant); THU (Therapeutic use); BIOL (Biological study); RACT (Reactant or reagent); USES (Uses)
(antiviral triaza compds., compns., and preparation)

10/680,076

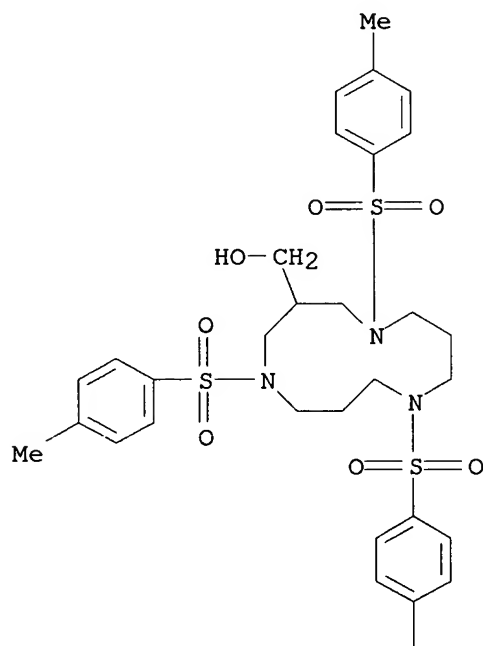
RN 182316-06-9 CAPLUS

CN 1,5,9-Triazacyclododecane, 3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]-
(9CI) (CA INDEX NAME)



RN 182316-17-2 CAPLUS

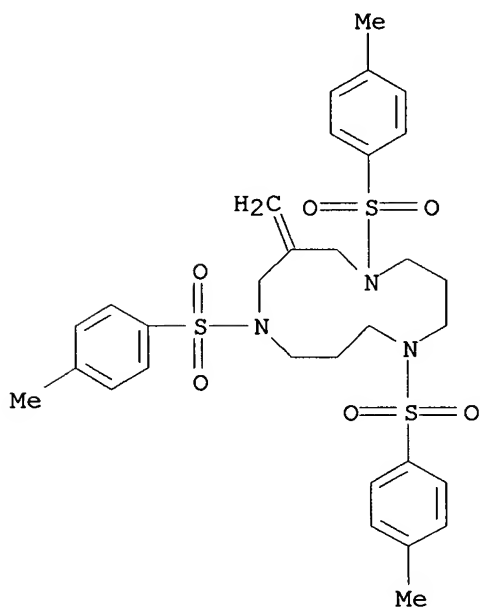
CN 1,5,9-Triazacyclododecane-3-methanol, 1,5,9-tris[(4-methylphenyl)sulfonyl]-
(9CI) (CA INDEX NAME)



PAGE 1-A

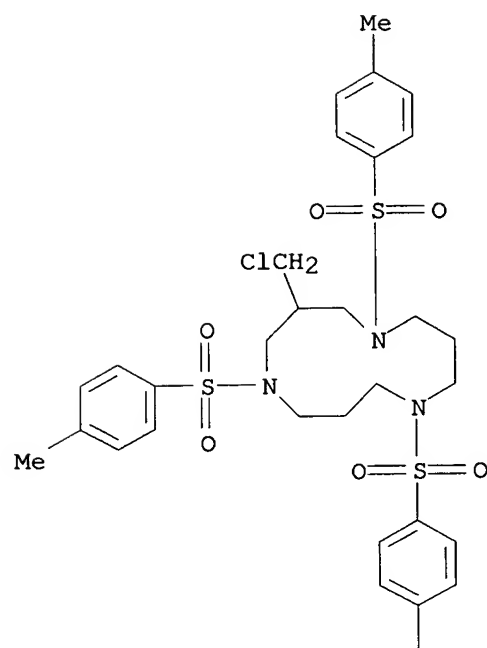
Me

IT 182316-15-0P 182316-19-4P 182316-22-9P
 182316-30-9P 182316-34-3P
 RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
 (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
 (Uses)
 (antiviral triaza compds., compns., and preparation)
 RN 182316-15-0 CAPLUS
 CN 1,5,9-Triazacyclododecane, 3-methylene-1,5,9-tris[(4-
 methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)



RN 182316-19-4 CAPLUS
 CN 1,5,9-Triazacyclododecane, 3-(chloromethyl)-1,5,9-tris[(4-
 methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)

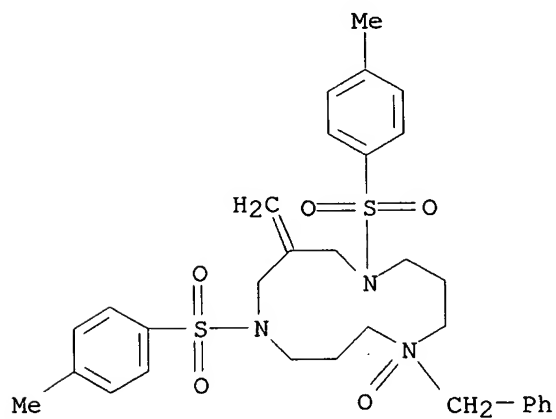
PAGE 1-A



PAGE 2-A

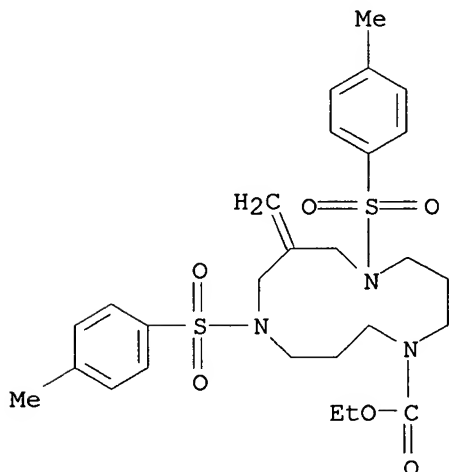


RN 182316-22-9 CAPLUS
 CN 1,5,9-Triazacyclododecane, 3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]-9-(phenylmethyl)-, 9-oxide (9CI) (CA INDEX NAME)



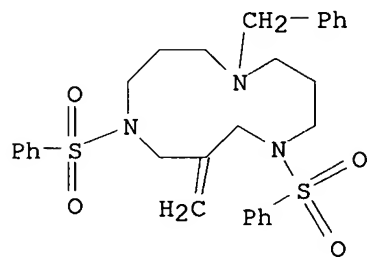
RN 182316-30-9 CAPLUS

CN 1,5,9-Triazacyclododecane-1-carboxylic acid, 7-methylene-5,9-bis[(4-methylphenyl)sulfonyl]-, ethyl ester (9CI) (CA INDEX NAME)



RN 182316-34-3 CAPLUS

CN 1,5,9-Triazacyclododecane, 3-methylene-9-(phenylmethyl)-1,5-bis(phenylsulfonyl)- (9CI) (CA INDEX NAME)



IT 182316-06-9D, derivs. 182316-08-1 182316-10-5

182316-12-7 182316-20-7 182316-21-8

182316-25-2 182316-27-4 182316-27-4D, acylated

392287-02-4 392287-03-5 392287-04-6

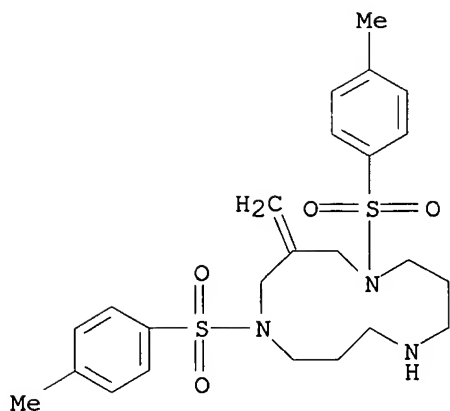
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL

(Biological study); USES (Uses)

(antiviral triaza compds., compns., and preparation)

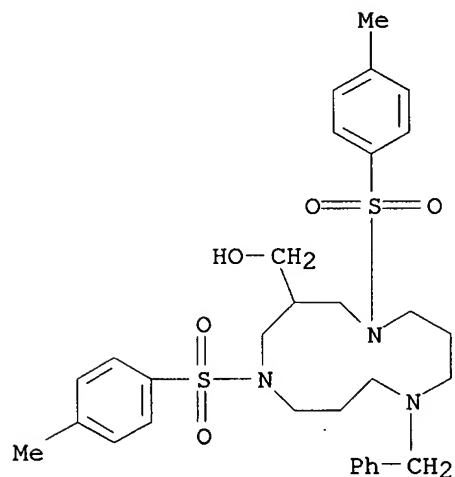
RN 182316-06-9 CAPLUS

CN 1,5,9-Triazacyclododecane, 3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)



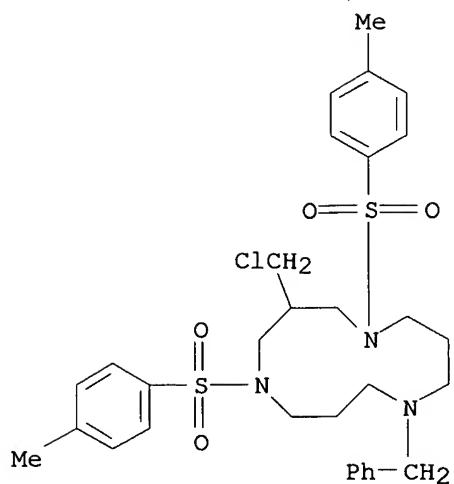
RN 182316-08-1 CAPLUS

CN 1,5,9-Triazacyclododecane-3-methanol, 1,5-bis[(4-methylphenyl)sulfonyl]-9-(phenylmethyl)- (9CI) (CA INDEX NAME)



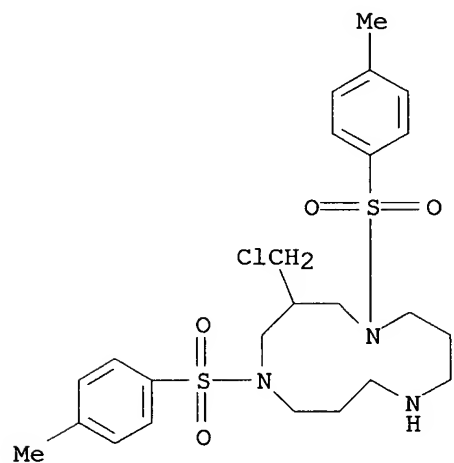
RN 182316-10-5 CAPLUS

CN 1,5,9-Triazacyclododecane, 3-(chloromethyl)-1,5-bis[(4-methylphenyl)sulfonyl]-9-(phenylmethyl)- (9CI) (CA INDEX NAME)



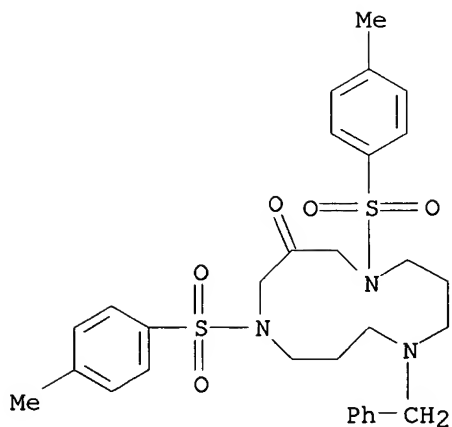
RN 182316-12-7 CAPLUS

CN 1,5,9-Triazacyclododecane, 3-(chloromethyl)-1,5-bis[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)



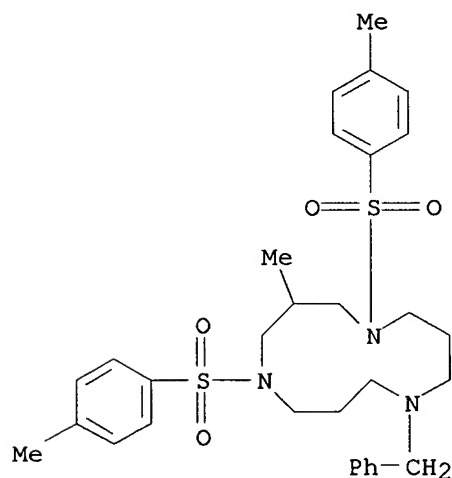
RN 182316-20-7 CAPLUS

CN 1,5,9-Triazacyclododecan-3-one, 1,5-bis[(4-methylphenyl)sulfonyl]-9-(phenylmethyl)- (9CI) (CA INDEX NAME)



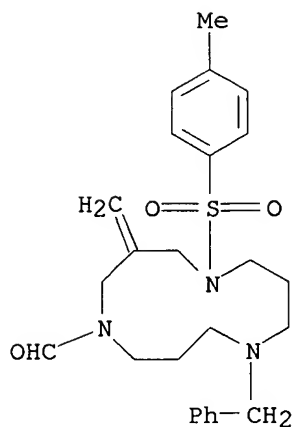
RN 182316-21-8 CAPLUS

CN 1,5,9-Triazacyclododecane, 3-methyl-1,5-bis[(4-methylphenyl)sulfonyl]-9-(phenylmethyl)- (9CI) (CA INDEX NAME)



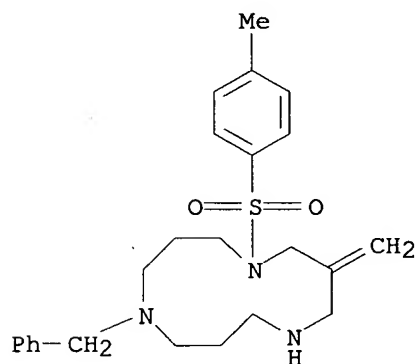
RN 182316-25-2 CAPLUS

CN 1,5,9-Triazacyclododecane-1-carboxaldehyde, 3-methylene-5-[(4-methylphenyl)sulfonyl]-9-(phenylmethyl)- (9CI) (CA INDEX NAME)



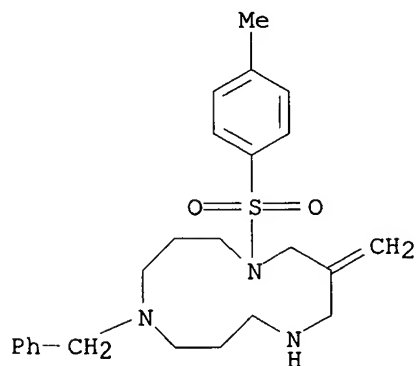
RN 182316-27-4 CAPLUS

CN 1,5,9-Triazacyclododecane, 3-methylene-1-[(4-methylphenyl)sulfonyl]-9-(phenylmethyl)- (9CI) (CA INDEX NAME)



RN 182316-27-4 CAPLUS

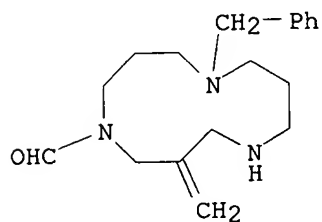
CN 1,5,9-Triazacyclododecane, 3-methylene-1-[(4-methylphenyl)sulfonyl]-9-(phenylmethyl)- (9CI) (CA INDEX NAME)



10/680,076

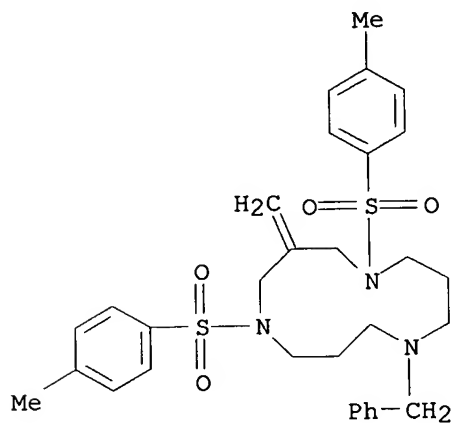
RN 392287-02-4 CAPLUS

CN 1,5,9-Triazacyclododecane-1-carboxaldehyde, 3-methylene-9-(phenylmethyl)-
(9CI) (CA INDEX NAME)



RN 392287-03-5 CAPLUS

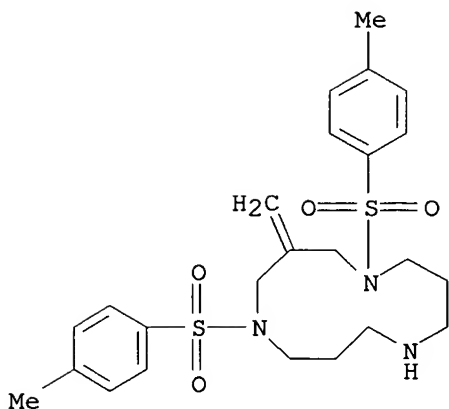
CN 1,5,9-Triazacyclododecane, 3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]-9-(phenylmethyl)-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

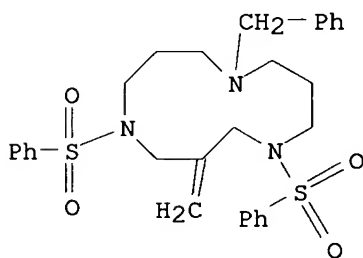
RN 392287-04-6 CAPLUS

CN 1,5,9-Triazacyclododecane, 3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]-,
monohydrochloride (9CI) (CA INDEX NAME)



● HCl

IT 182316-50-3P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (antiviral triaza compds., compns., and preparation)
 RN 182316-50-3 CAPLUS
 CN 1,5,9-Triazacyclododecane, 3-methylene-9-(phenylmethyl)-1,5-
 bis(phenylsulfonyl)-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

30 ANSWER 18 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2001:218085 CAPLUS

DOCUMENT NUMBER: 135:5605

TITLE: Synthesis of Polyazamacrocyclic Compounds via Modified Richman-Atkins Cyclization of β -Trimethylsilylethanesulfonamides

AUTHOR(S): Hoyer, Rebecca C.; Richman, Jack E.; Dantas, Gautam A.; Lightbourne, Marissa F.; Shinneman, L. Scott

CORPORATE SOURCE: Department of Chemistry, Macalester College, St. Paul, MN, 55105, USA

SOURCE: Journal of Organic Chemistry (2001), 66(8), 2722-2725
CODEN: JOCEAH; ISSN: 0022-3263

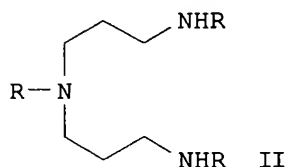
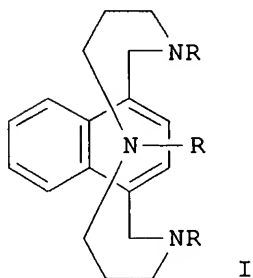
PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 135:5605

GI



AB The use of β -trimethylsilylethanesulfonamides (SES-sulfonamides) for the preparation of polyazamacrocyclic compds. is described. This expands existing Richman-Atkins sulfonamide macrocyclization methodol., and it successfully enables preparation of labile polyaza[n](1,4)naphthalenophanes and polyaza[n](9,10)anthracenophanes, not previously available in appreciable quantities. Thus, triazanaphthalenecyclophane I ($R = \text{Me}_3\text{SiCH}_2\text{CH}_2\text{SO}_2$) was prepared from 1,4-bis(bromomethyl)naphthalene and the trimethylethanesulfonamide II.

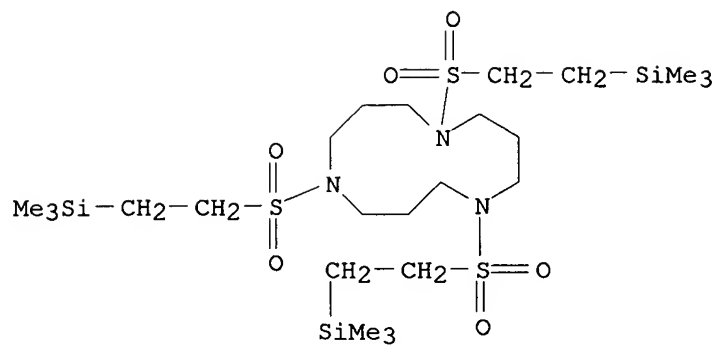
IT 340970-56-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of azacyclophanes via Richman-Atkins cyclization of trimethylsilylethanesulfonamides with ditosylates or bis(bromomethyl) compds.)

RN 340970-56-1 CAPLUS

CN 1,5,9-Triazacyclododecane, 1,5,9-tris[[2-(trimethylsilyl)ethyl]sulfonyl]-(9CI) (CA INDEX NAME)



REFERENCE COUNT: 43 THERE ARE 43 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

10/680,076

~~L80~~ ANSWER 19 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2001:107172 CAPLUS

DOCUMENT NUMBER: 134:277328

TITLE: Remarkable cooperative action of two zinc centers in the hydrolysis of plasmid DNA

AUTHOR(S): Aka, F. Nihan; Akkaya, Mahinur S.; Akkaya, Engin U.

CORPORATE SOURCE: Department of Chemistry, Middle East Technical University, Ankara, TR-06531, Turk.

SOURCE: Journal of Molecular Catalysis A: Chemical (2001), 165(1-2), 291-294

CODEN: JMCCF2; ISSN: 1381-1169

PUBLISHER: Elsevier Science B.V.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB A novel binuclear zinc complex has been synthesized. The complex is highly efficient in the hydrolysis of plasmid DNA at pH 7.5. Furthermore, a comparison to a mononuclear complex reveals a high level of cooperativity between the two metal ion centers.

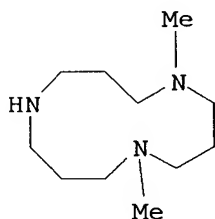
IT 139258-69-8

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); BIOL (Biological study); RACT (Reactant or reagent)

(preparation and DNA hydrolytic activity of binuclear zinc complex)

RN 139258-69-8 CAPLUS

CN 1,5,9-Triazacyclododecane, 1,5-dimethyl- (9CI) (CA INDEX NAME)



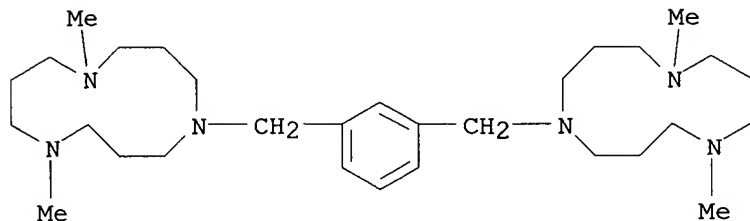
IT 333784-11-5P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and DNA hydrolytic activity of binuclear zinc complex)

RN 333784-11-5 CAPLUS

CN 1,5,9-Triazacyclododecane, 1,1'-[1,3-phenylenebis(methylene)]bis[5,9-dimethyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT:

35

THERE ARE 35 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

~~130~~ ANSWER 20 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2001:69121 CAPLUS

DOCUMENT NUMBER: 134:131928

TITLE: Epoxidation catalysts and production method of epoxidized compounds of olefins therewith

INVENTOR(S): Sakamoto, Takaki; Park, Chong Jin

PATENT ASSIGNEE(S): Kawamura Institute of Chemical Research, Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 9 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2001025665	A2	20010130	JP 1999-202402	19990716
PRIORITY APPLN. INFO.:			JP 1999-202402	19990716

AB Title catalysts comprise (1) methyltrioxorhenium (CH₃ReO₃) and (2) cyclic triamines selected from 1,4,7-trimethyl-1,4,7-triazacyclononane, 1,4,7-triethyl-1,4,7-triazacyclononane, 1,4,7-tripropyl-1,4,7-triazacyclononane, 1,5,9-trimethyl-1,5,9-triazacyclododecane, 1,5,9-triethyl-1,5,9-triazacyclododecane, and 1,5,9-tripropyl-1,5,9-triazacyclododecane on supports selected from alumina, silica gel, and florisil. Thus, 0.246 g cyclohexane was reacted with 0.68 g 30% H₂O₂ in water in the presence of a catalyst comprising methyltrioxorhenium 250, 1,4,7-trimethyl-1,4,7-triazacyclononane 171, and silica gel 500 mg to give a cyclohexane oxide with conversion rate and selectivity 100%.

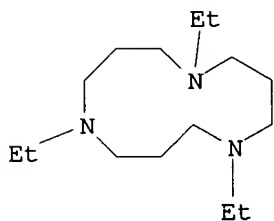
IT 321861-36-3 321861-37-4

RL: CAT (Catalyst use); USES (Uses)

(epoxidn. catalysts for preparation of epoxy compds. from olefins)

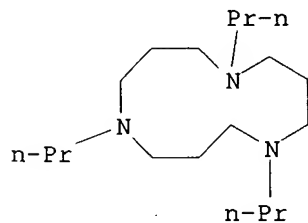
RN 321861-36-3 CAPLUS

CN 1,5,9-Triazacyclododecane, 1,5,9-triethyl- (9CI) (CA INDEX NAME)



RN 321861-37-4 CAPLUS

CN 1,5,9-Triazacyclododecane, 1,5,9-tripropyl- (9CI) (CA INDEX NAME)



100 ANSWER 21 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2000:695769 CAPLUS

DOCUMENT NUMBER: 133:355853

TITLE: Mn²⁺, Co²⁺, Cu²⁺ and Zn²⁺ complexes with two macrocyclic ligands bearing L-lactate-like functions: potentiometric studies and evaluation of

AUTHOR(S): superoxide-scavenging properties of the Mn²⁺ complex
 CORPORATE SOURCE: Delagrangé, Samuel; Delgado, Rita; Nepveu, Françoise
 Laboratoire Pharmacophores Redox, Phytochimie et Radiobiologie, Université Paul Sabatier 35, Toulouse, 31062, Fr.

SOURCE: Journal of Inorganic Biochemistry (2000), 81(1-2), 65-71

CODEN: JIBIDJ; ISSN: 0162-0134

PUBLISHER: Elsevier Science Inc.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Some aerobic organisms devoid of SOD use Mn²⁺ chelates to scavenge the O₂-radical. Since the Mn²⁺-bis(lactato)diaquo complex is known as having a high SOD-like activity, the authors prepared manganese(II) complexes with triazamacrocyclic ligands bearing L-lactate-like functions to obtain model compds. able to disproportionate the superoxide radical. Thus, two macrocyclic ligands, N,N',N''-tris[2(S)-hydroxybutyric acid]-1,4,7-triazacyclononane, L1, and N,N',N''-tris[2(S)-hydroxybutyric acid]-1,5,9-triazacyclododecane, L2, were prepared (prior work) and their capacity to retain the Mn²⁺ ion in aqueous solution was determined from potentiometric

expts. The chelating properties in aqueous solution of each ligand towards Co²⁺,

Cu²⁺ and Zn²⁺ ions were also determined. L1 forms complexes with Mn²⁺, Co²⁺, Cu²⁺ and Zn²⁺ ions with stability consts. of 8.33(5), 15.78(5), 17.65(3) and 14.32(1), resp. L2 forms complexes with Cu²⁺ and Zn²⁺ ions with stability consts. of 10.67(1) and 6.98(3), resp. But the consts. related to the Mn²⁺ and Co²⁺ complexes were too low to be determined by the method used. The stability consts. values calculated for L2 complexes are significantly lower than those for the corresponding complexes of L1. Addnl. spectroscopic measurements were carried out on the Mn²⁺-L1 system. The electronic spectrum of this system showed a pH-dependence that may be consistent with the formation of hydroxo-species as the ESR spectra recorded at 120 K did not show oxidation of the Mn²⁺ ion in the pH range studied. The superoxide-scavenging activity of the manganese(II)-L1 complex was investigated using the cytochrome c assay. The Mn²⁺-L1 system showed an IC₅₀ value of 1.7 µM which indicates that it appears as a potent SOD mimic.

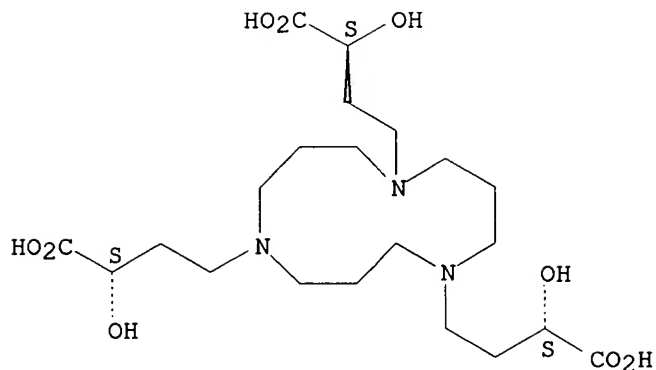
IT 241486-68-0

RL: PRP (Properties); RCT (Reactant); RACT (Reactant or reagent)
 (protonation consts. and complexation with transition metals)

RN 241486-68-0 CAPLUS

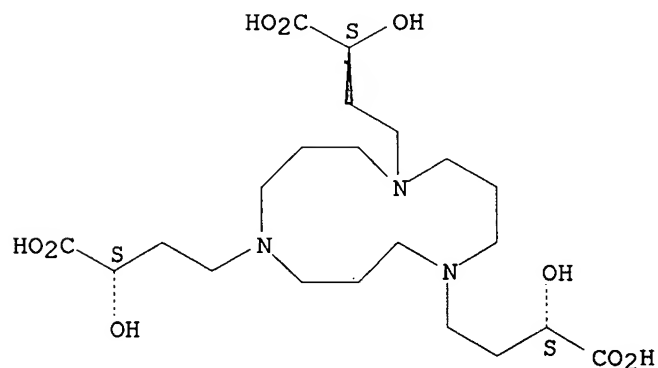
CN 1,5,9-Triazacyclododecane-1,5,9-tributanoic acid,
 α,α',α''-trihydroxy-, (αS,α'S,α''S)-
 (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 241486-68-0D, copper and zinc complexes
 RL: CAT (Catalyst use); FMU (Formation, unclassified); PRP (Properties);
 FORM (Formation, nonpreparative); USES (Uses)
 (stability consts.)
 RN 241486-68-0 CAPLUS
 CN 1,5,9-Triazacyclododecane-1,5,9-tributanoic acid,
 $\alpha, \alpha', \alpha''$ -trihydroxy-, ($\alpha S, \alpha' S, \alpha'' S$)-
 (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 28 THERE ARE 28 CITED REFERENCES AVAILABLE FOR THIS
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

~~130~~ ANSWER 22 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2000:554692 CAPLUS

DOCUMENT NUMBER: 133:275527

TITLE: Ligand Macrocyclic Structural Effects on Copper-Dioxygen Reactivity

AUTHOR(S): Lam, Bernice M. T.; Halfen, Jason A.; Young, Victor G., Jr.; Hagadorn, John R.; Holland, Patrick L.; Lledos, Agusti; Cucurull-Sanchez, Lourdes; Novoa, Juan J.; Alvarez, Santiago; Tolman, William B.

CORPORATE SOURCE: Department of Chemistry and Center for Metals in Biocatalysis, University of Minnesota, Minneapolis, MN, 55455, USA

SOURCE: Inorganic Chemistry (2000), 39(18), 4059-4072
CODEN: INOCAJ; ISSN: 0020-1669

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB With the goal of understanding how the nature of the tridentate macrocyclic supporting ligand influences the relative stability of isomeric μ - η^2 : η^2 -peroxo- and bis(μ -oxo)dicopper complexes, a comparative study was undertaken of the O₂ reactivity of Cu(I) compds. supported by the 10- and 12-membered macrocycles, 1,4,7-R₃-1,4,7-triazacyclododecane (R₃TACD; R = Me, Bn, iPr) and 1,5,9-triisopropyl-1,5,9-triazacyclododecane (iPr₃TACDD). While the 3-coordinate complex [(iPr₃TACDD)Cu]SbF₆ was unreactive with O₂, oxygenation of [(R₃TACD)Cu(MeCN)]X (R = Me or Bn; X = ClO₄⁻ or SbF₆⁻) at -80° yielded bis(μ -oxo) species [(R₃TACD)₂Cu₂(μ -O)₂]X₂ as revealed by UV-visible and resonance Raman spectroscopy. Interestingly, unlike the previously reported system supported by 1,4,7-triisopropyl-1,4,7-triazacyclononane (iPr₃TACN), which yielded interconverting mixts. of peroxo and bis(μ -oxo) compds. (Cahoy, J.; Holland, P. L.; Tolman, W. B. Inorg. Chemical 1999, 38, 2161), low-temperature oxygenation of [(iPr₃TACD)Cu(MeCN)]SbF₆ in a variety of solvents cleanly yielded a μ - η^2 : η^2 -peroxo product, with no trace of the bis(μ -oxo) isomer. The peroxo complex was characterized by UV-visible and resonance Raman spectroscopy, as well as an x-ray crystal structure (albeit of marginal quality due to disorder problems). Intramol. attack at the α C-H bonds of the substituents was indicated as the primary decomposition pathway of the oxygenated compds. through examination of the decay

kinetics and the reaction products, which included bis(μ -hydroxo)- and μ -carbonato-dicopper complexes that were characterized by x-ray diffraction. A rationale for the varying results of the oxygenation reactions was provided by anal. of (a) the x-ray crystal structures and electrochem. behavior of the Cu(I) precursors and (b) the results of theor. calcns. of the complete oxygenated complexes, including all ligand atoms, using combined quantum chemical/mol. mechanics (integrated MO mol. mechanics, IMOMM) methods. The size of the ligand substituents is a key factor in controlling the relative stabilities of the peroxo and bis(μ -oxo) forms, and the nature of this influence was shown by both theory and experiment to depend on the ligand macrocycle ring size.

IT 296761-76-7P, 1,5,9-Triisopropyl-1,5,9-triazacyclododecane
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

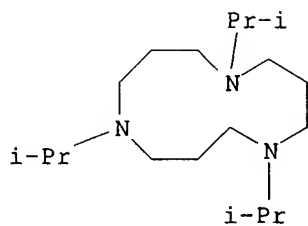
(preparation, complexation with copper(I), and influence of ring size on copper-dioxygen reactivity)

RN 296761-76-7 CAPLUS

CN 1,5,9-Triazacyclododecane, 1,5,9-tris(1-methylethyl)- (9CI) (CA INDEX

10/680,076

NAME)



REFERENCE COUNT:

77

THERE ARE 77 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

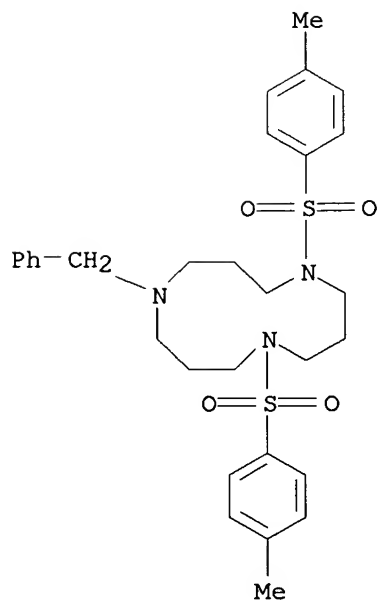
~~L70~~ ANSWER 23 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2000:165352 CAPLUS
DOCUMENT NUMBER: 132:321849
TITLE: Multi-layer macromonocyclic polyamines. I. Molecular
design and synthesis of component monocyclic
precursors
AUTHOR(S): Iwata, Masaaki
CORPORATE SOURCE: Biopolymer Phys. Lab., The Institute of Physical and
Chemical Research (RIKEN), Wako, Saitama, 351-0198,
Japan
SOURCE: Bulletin of the Chemical Society of Japan (2000),
73(3), 693-704
CODEN: BCSJA8; ISSN: 0009-2673
PUBLISHER: Chemical Society of Japan
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 132:321849
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Multi-layer macromonocyclic polyamines, which might be appropriate
polymorphismic mol. scaffolds as host-mols. in ionic or mol. interaction
with small or large guest ions or mols, have been designed. In
polymorphismic mols., several macromonocyclic polyamines with the same
and/or different ring sizes and nitrogen contents are connected to each
other by alkylene spacers with various length of chain. Actual target
mols. were characterized by possessing methylene chain arrays of natural
polyamines. Fourteen component macromonocycles of various sizes, e.g. 12-
to 34-membered rings containing three to eight nitrogen atoms, were prepared
from simple starting materials as essential building blocks required for
construction of multi-layer mols. The synthetic method was very
efficient. In a final step, the N-protecting benzyl group was
successfully removed by hydrogenation on 10%-Pd/C under 4 kg cm⁻² H₂ to
give the cyclic amine precursors, e.g. I and II, which could be internal
and terminal components in the architecture of the multi-layer mols. The
structures of synthesized compds. were characterized and confirmed by
elemental anal., ¹H-NMR, and SIMS and FAB(+) mass spectrometry.

IT 164913-15-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(preparation of macromonocyclic polyamines and mol. design of multi-layer
macromonocyclic polyamines)

RN 164913-15-9 CAPLUS
CN 1,5,9-Triazacyclododecane, 1,5-bis[(4-methylphenyl)sulfonyl]-9-
(phenylmethyl)- (9CI) (CA INDEX NAME)



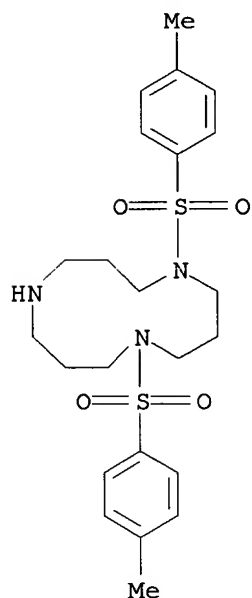
IT 164913-31-9P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of macromonocyclic polyamines and mol. design of multi-layer macromonocyclic polyamines)

RN 164913-31-9 CAPLUS

CN 1,5,9-Triazacyclododecane, 1,5-bis[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)



REFERENCE COUNT:

45

THERE ARE 45 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

~~130~~ ANSWER 24 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2000:119093 CAPLUS

DOCUMENT NUMBER: 132:216106

TITLE: The first dicopper(II) complex of a new bis(1,5,9-triazacyclododecane) ligand: synthesis, crystal structure and magnetic coupling of the complex

AUTHOR(S): Bu, Xian-He; Lu, Shou-Liang; Zhang, Ruo-Hua; Liao, Dai-Zheng; Aoki, Shin; Clifford, Thomas; Kimura, Eiichi

CORPORATE SOURCE: Department of Chemistry, Nankai University, Tianjin, 300071, Peop. Rep. China

SOURCE: Inorganica Chimica Acta (2000), 298(1), 50-56
CODEN: ICHAA3; ISSN: 0020-1693

PUBLISHER: Elsevier Science S.A.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB A new binucleating macrocyclic polyamine ligand based on 1,5,9-triazacyclododecane ([12]aneN3), 2,6-bis(1,5,9-triazacyclododecan-9-ylmethyl)benzoic acid (HL), was synthesized from a selectively Boc protected [12]aneN3 precursor and 2,6-bis(bromomethyl) benzoate. L can form a stable binuclear complex with Cu(II) in aqueous solution,

[Cu₂L(N₃)₂]ClO₄, which was characterized by x-ray crystallog. (monoclinic, space group Cc, R = 0.069). The intramol. binuclear Cu(II) centers are bridged by a μ -carboxyl group on L and separated by 5.947 Å. Both of the Cu(II) centers are coordinated by three amine nitrogens of [12]aneN3 subunit and one oxygen of the carboxyl group, as well as one azide anion, and each Cu(II) center is in a distorted state intermediate between a square-pyramid and trigonal-bipyramid environment. This is the 1st binuclear Cu(II) complex formed with a bis([12]aneN3) ligand. Variable temperature magnetic susceptibility studies indicate that there exists intramol.

antiferromagnetic coupling ($-2J = 71.4 \text{ cm}^{-1}$) between the two unpaired electrons of the two Cu(II) ions in the complex.

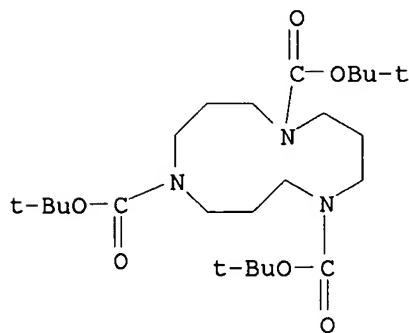
IT 260433-36-1P, 1,5,9-Tris(N-tert-butoxycarbonyl)-1,5,9-triazacyclododecane

RL: BYP (Byproduct); PREP (Preparation)

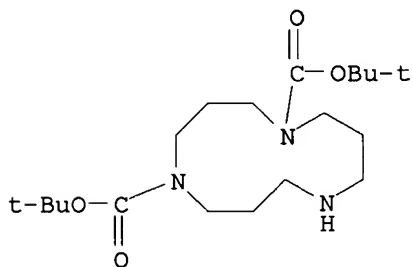
(byproduct in preparation of copper(II) bis(triazacyclododecan-9-ylmethyl)benzoato azido dinuclear complex)

RN 260433-36-1 CAPLUS

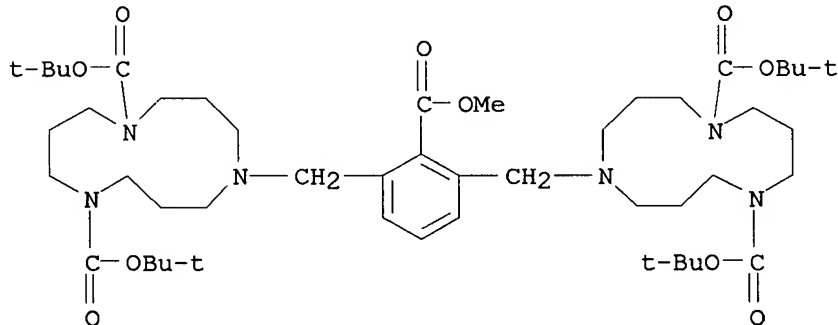
CN 1,5,9-Triazacyclododecane-1,5,9-tricarboxylic acid, tris(1,1-dimethylethyl) ester (9CI) (CA INDEX NAME)



IT 174192-40-6P, 1,5-Bis(N-tert-butoxycarbonyl)-1,5,9-triazacyclododecane 260433-33-8P, Methyl 2,6-bis(1,5-bis(N-tert-butoxycarbonyl)-1,5,9-triazacyclododecan-9-ylmethyl)benzoate
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (for preparation of copper(II) bis(triazacyclododecanylmethyl)benzoato azido dinuclear complex)
 RN 174192-40-6 CAPLUS
 CN 1,5,9-Triazacyclododecane-1,5-dicarboxylic acid, bis(1,1-dimethylethyl) ester (9CI) (CA INDEX NAME)



RN 260433-33-8 CAPLUS
 CN 1,5,9-Triazacyclododecane-1,5-dicarboxylic acid, 9,9'-[[2-(methoxycarbonyl)-1,3-phenylene]bis(methylene)]bis-, tetrakis(1,1-dimethylethyl) ester (9CI) (CA INDEX NAME)



REFERENCE COUNT:

46

THERE ARE 46 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

~~LEO~~ ANSWER 25 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1999:777516 CAPLUS

DOCUMENT NUMBER: 132:137370

TITLE: Application of matrix-assisted laser desorption/ionization time-of-flight mass spectrometry to the structure determination of medium and large macrocycles formed by palladium(0)-catalyzed allylation of arenesulfonamides, sulfamide, and cyanamide

AUTHOR(S): Cerezo, Silvia; Cortes, Jordi; Galvan, David; Lopez-Romero, Juan-Manuel; Moreno-Manas, Marcial; Pleixats, Roser; Aviles, Francesc X.; Canals, Francesc; Roglans, Anna

CORPORATE SOURCE: Department of Chemistry, Universitat Autònoma de Barcelona, Barcelona, 08193, Spain

SOURCE: Rapid Communications in Mass Spectrometry (1999), 13(23), 2359-2365

CODEN: RCMSEF; ISSN: 0951-4198

PUBLISHER: John Wiley & Sons Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Matrix-assisted laser desorption/ionization time-of-flight mass spectrometry allowed the direct determination of the extent of macrocyclic and linear oligomer formation in the palladium(0)-catalyzed allylation of highly acidic and non-nucleophilic arenesulfonamides, sulfamide, and cyanamide. Palladium-containing 15-membered-ring macrocyclic compds. gave unusual $[M - H]^+$ ions besides $[M + Na]^+$ and $[M + K]^+$ adducts.

IT 130927-35-4 219839-43-7 219839-47-1
219839-49-3

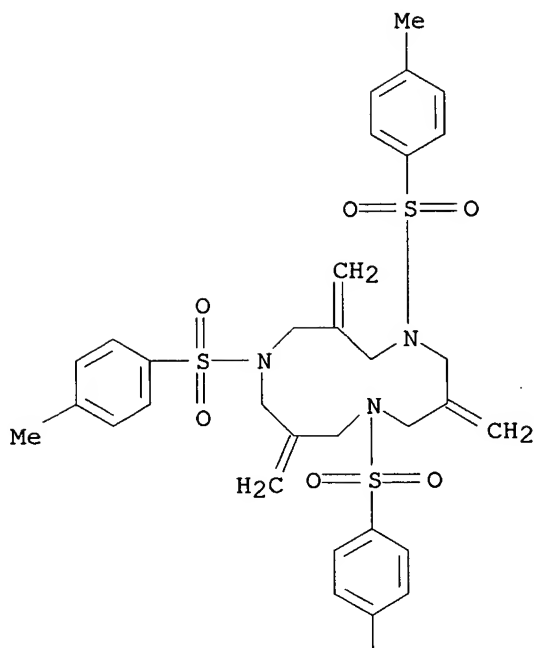
RL: PRP (Properties)

(structure determination by MALDI-TOF mass spectrometry of cyclic compds. formed by palladium(0)-catalyzed allylation of arenesulfonamides, sulfamide, and cyanamide)

RN 130927-35-4 CAPLUS

CN 1,5,9-Triazacyclododecane, 3,7,11-tris(methylene)-1,5,9-tris[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)

PAGE 1-A

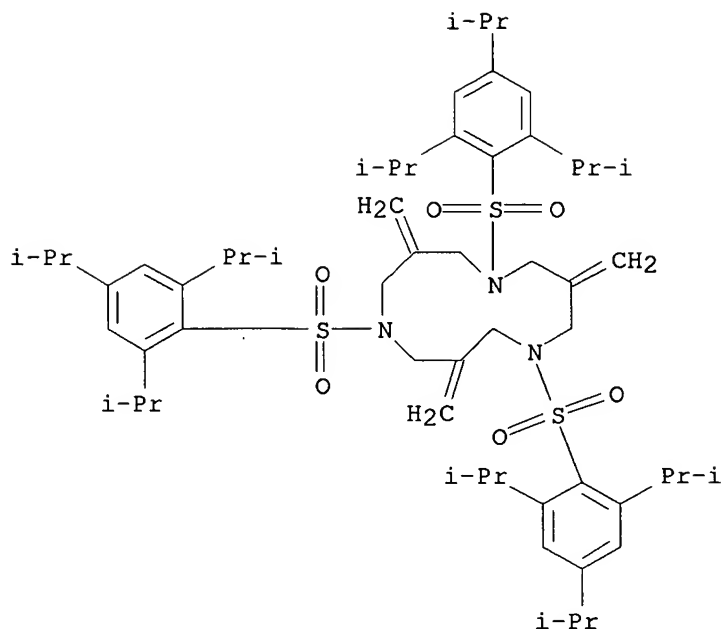


PAGE 2-A



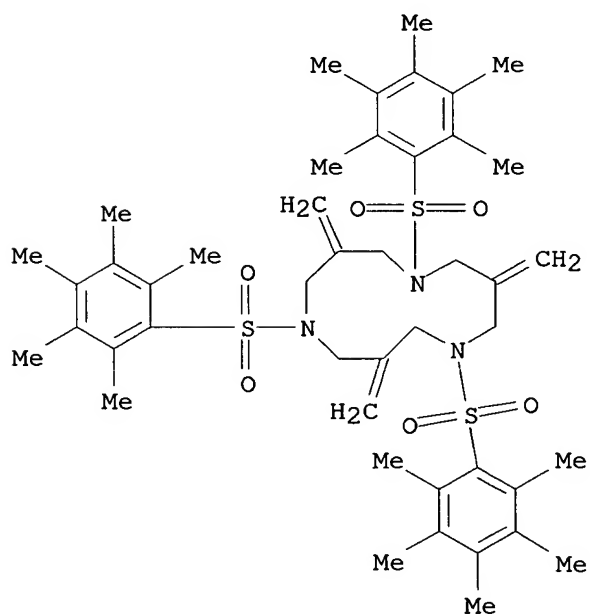
RN 219839-43-7 CAPLUS

CN 1,5,9-Triazacyclododecane, 3,7,11-tris(methylene)-1,5,9-tris[[2,4,6-tris(1-methylethyl)phenyl]sulfonyl]- (9CI) (CA INDEX NAME)



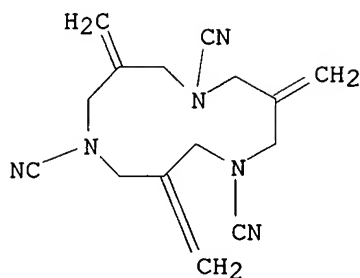
RN 219839-47-1 CAPLUS

CN 1,5,9-Triazacyclododecane, 3,7,11-tris(methylene)-1,5,9-tris[(pentamethylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)



RN 219839-49-3 CAPLUS

CN 1,5,9-Triazacyclododecane-1,5,9-tricarbonitrile, 3,7,11-tris(methylene)- (9CI) (CA INDEX NAME)

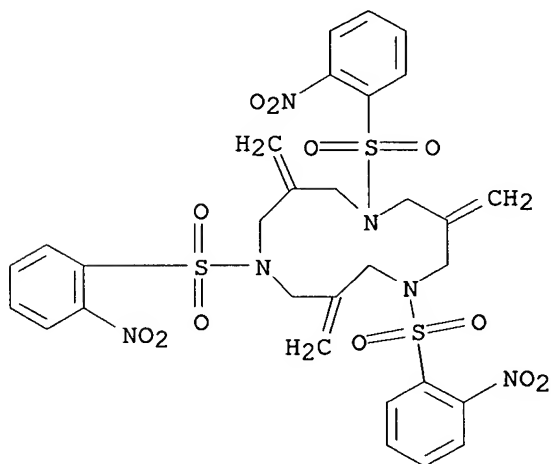


IT 256498-09-6P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
 (structure determination by MALDI-TOF mass spectrometry of cyclic compds.
 formed by palladium(0)-catalyzed allylation of arenesulfonamides,
 sulfamide, and cyanamide)

RN 256498-09-6 CAPLUS

CN 1,5,9-Triazacyclododecane, 3,7,11-tris(methylene)-1,5,9-tris[(2-
 nitrophenyl)sulfonyl]- (9CI) (CA INDEX NAME)



REFERENCE COUNT:

20

THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L30 ANSWER 26 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1999:752089 CAPLUS

DOCUMENT NUMBER: 132:3924

TITLE: Artificial leather sheets with good embossability and manufacture therewith

INVENTOR(S): Ikebukuro, Kazunari; Wakamatsu, Tomoyuki

PATENT ASSIGNEE(S): Kuraray Co., Ltd., Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 8 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

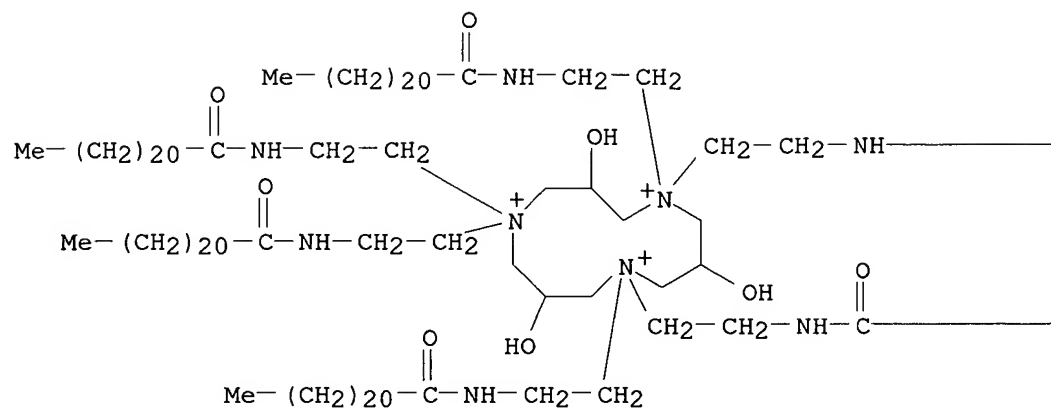
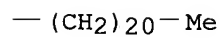
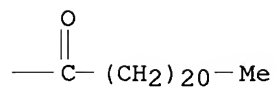
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 11323742	A2	19991126	JP 1998-137300	19980520
PRIORITY APPLN. INFO.:			JP 1998-137300	19980520

AB The manufacture includes imparting a cationic surfactant onto a nonporous layer-covered fiber base layer and subjecting to the embossment treatment, where the nonporous layer consists of a diamine- or hydrazide-extended aliphatic or alicyclic polyurethane elastomer or a diol-extended MDI-type polyurethane elastomer. Coating a DMF solution of polyurethane elastomer (PUE) consisting of poly(ethylene adipate) glycol (I), 4,4'-MDI, ethylene glycol on a polyethylene film, coagulation in aqueous DMF, removing polyethylene film, and bonding the resulting porous film with a polyester fabric gave a base. Coating sequentially the base on the porous film with a polyurethane consisting of I, cyclohexylmethane-4,4'-diisocyanate, and isophoronediamine and PUE, treating with 1,5,9-Triazoniacyclododecane derivative cation [(C₂₁H₄₃CONHCH₂CH₂)₂N+CH₂CHOHCH₂]^{3.3} Cl⁻ and embossing gave a leather-like sheet with good appearance.

IT 137955-63-6
 RL: TEM (Technical or engineered material use); USES (Uses)
 (artificial leather sheets with good embossability and manufacture therewith)

RN 137955-63-6 CAPLUS

CN 1,5,9-Triazoniacyclododecane, 3,7,11-trihydroxy-1,1,5,5,9,9-hexakis[2-[(1-oxodocosyl)amino]ethyl]-, trichloride (9CI) (CA INDEX NAME)

● 3 Cl^- 

130 ANSWER 27 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1999:700785 CAPLUS

DOCUMENT NUMBER: 132:61413

TITLE: Molecular recognition of synthetic siderophore analogues: a study with receptor-deficient and fhu(A-B) deletion mutants of *Escherichia coli*

AUTHOR(S): Gaspar, Margarida; Santos, M. Amelia; Krauter, Katja; Winkelmann, Gunther

CORPORATE SOURCE: Centro de Quimica Estrutural, Complexo I, Instituto Superior Tecnico, Lisbon, 1049-001, Port.

SOURCE: BioMetals (1999), 12(3), 209-218

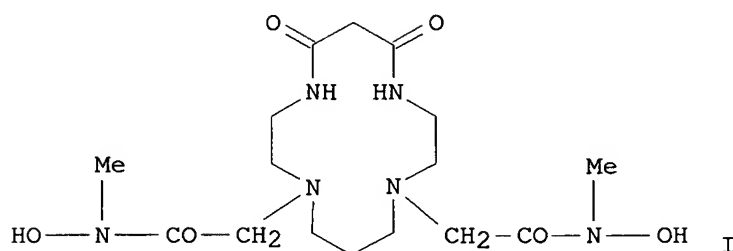
CODEN: BOMEEH; ISSN: 0966-0844

PUBLISHER: Kluwer Academic Publishers

DOCUMENT TYPE: Journal

LANGUAGE: English

GI



AB The biol. activity of six synthetic siderophore analogs [two dihydroxamates, two trihydroxamates, one tetrahydroxamate and one 3-hydroxy-4(1H)pyridinone] has been studied in *Escherichia coli*, *Morganella morganii* 13 and *Proteus mirabilis* 8993 strains by using growth promotion tests. Various transport-deficient mutants of *E. coli* were used to study the route of entry into gram-neg. bacteria. The results indicated that the synthetic hydroxamate compds. are transported via Fhu-mediated transport systems, although receptor specificity was low. This could be proven by using a delta (fhuA-B) *E. coli* mutant as a control in which growth promotion by natural hydroxamates was completely abolished, suggesting that a periplasmic binding-protein-dependent transport system (FhuB, C, D) is required for the transport of all synthetic ferric hydroxamate complexes. Although utilization of the synthetic hydroxamates was generally lower than that of the natural siderophores, differences in growth promotion could be detected. Highest activity was observed with the dihydroxamate DOCYDHAMA (I) ligand which supported growth at concns. <1 mM. In comparison with other polyamino-polyhydroxamate ligands studied, I has an extra diamide backbone that could be important for the interaction with the receptors or with FhuD. The synthetic trihydroxamate and tetrahydroxamate ligands showed a relatively low siderophore activity. Studies with *Proteus* and *Morganella* in the presence of increasing bipyridyl concns. showed a decreased growth promotion with the synthetic ferric hydroxamates, suggesting the involvement of a reduction step during iron mobilization or an increased toxicity of bipyridyl. This was not observed in the case of the 3-hydroxy-4(1H)pyridinone where bipyridyl had no effect.

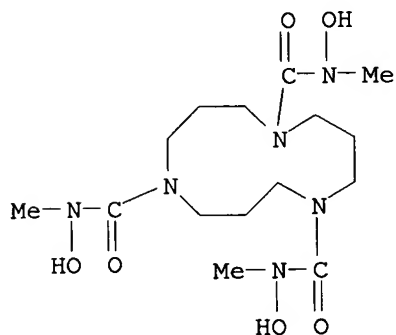
IT 169386-06-5

RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL

(Biological study); PROC (Process)

(mol. recognition of synthetic siderophore analogs studied with
transport-deficient mutants of *Escherichia coli*)

RN 169386-06-5 CAPLUS

CN 1,5,9-Triazacyclododecane-1,5,9-tricarboxamide, N,N',N''-trihydroxy-
N,N',N''-trimethyl- (9CI) (CA INDEX NAME)

REFERENCE COUNT:

33

THERE ARE 33 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

~~130~~ ANSWER 28 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1999:631224 CAPLUS

DOCUMENT NUMBER: 131:279208

TITLE: Methine compound for silver halide photographic material

INVENTOR(S): Kato, Takashi

PATENT ASSIGNEE(S): Fuji Photo Film Co., Ltd., Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 23 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 11269398	A2	19991005	JP 1998-70936	19980319
PRIORITY APPLN. INFO.:			JP 1998-70936	19980319

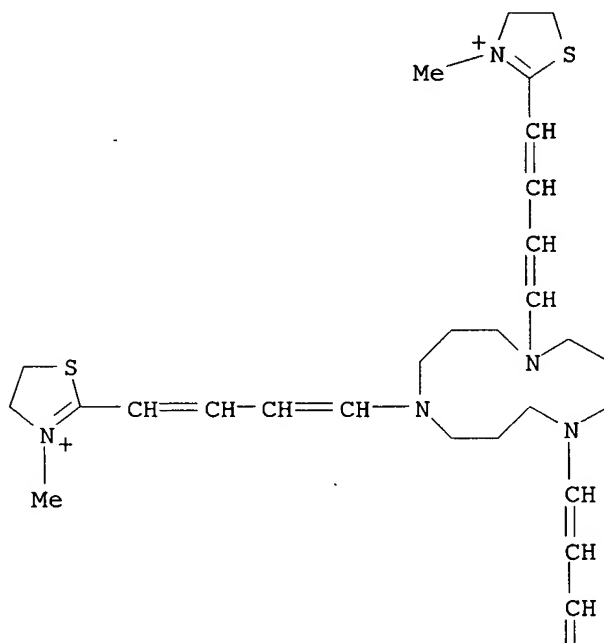
AB The methine compound of a polymer hemicyanine has structure
H1-A1-(-H2-A2-)q1-H3(H1-3 = hemicyanine dye; A1-2 = connecting group; q1
= 2-10,000 integer). The methine compound provides the improved
sensitivity.

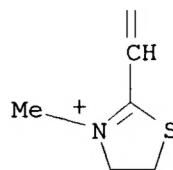
IT 245342-46-5
RL: TEM (Technical or engineered material use); USES (Uses)
(methine compound for silver halide photog. material)

RN 245342-46-5 CAPLUS

CN Thiazolium, 2,2',2''-(1,5,9-triazacyclododecane-1,5,9-triyltri-1,3-
butadiene-4,1-diyl)tris[4,5-dihydro-3-methyl-, tribromide (9CI) (CA INDEX
NAME)

PAGE 1-A





●3 Br⁻

130 ANSWER 29 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1999:475681 CAPLUS

DOCUMENT NUMBER: 131:308148

TITLE: Polyamino-polyhydroxamic acids as siderophore analogs

AUTHOR(S): Santos, M. Amelia

CORPORATE SOURCE: Centro de Quimica Estrutural, Instituto Superior Tecnico, Lisbon, 1049-001, Port.

SOURCE: Monograph Series of the International Conferences on Coordination Chemistry held periodically at Smolenice in Slovakia (1999), 4 (Coordination Chemistry at the Turn of the Century), 327-332
CODEN: MSICF5; ISSN: 1335-308X

PUBLISHER: Slovak Technical University Press

DOCUMENT TYPE: Journal

LANGUAGE: English

AB This paper presents a synopsis of the study of a set of polyamino-polyhydroxamate ligands as potential analogs of naturally occurring hydroxamate siderophores. They all have a cyclic (or macrocyclic) polyamine backbone with two or three hydroxamate pendant groups attached to the amine sites. Most of them are biol. active. They have been prepared by procedures which are schematically presented herein. Particular emphasis is devoted to their interaction with iron(III), namely what concerns the stability of the ferric complexes (Fe2L3 or FeL), their redox potentials, and the speciation at physiol. pH. Proposed structures of the dimeric complexes are supported by mol. modeling calcns. A summary of the in vivo studies is also presented. Comparison between the properties of the iron complexes and some siderophores is also made.

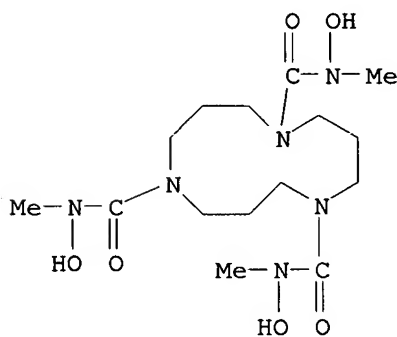
IT 169386-06-5P 247912-38-5P

RL: BAC (Biological activity or effector, except adverse); BPR (Biological process); BSU (Biological study, unclassified); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); PROC (Process)

(polyamino-polyhydroxamic acids as siderophore analogs)

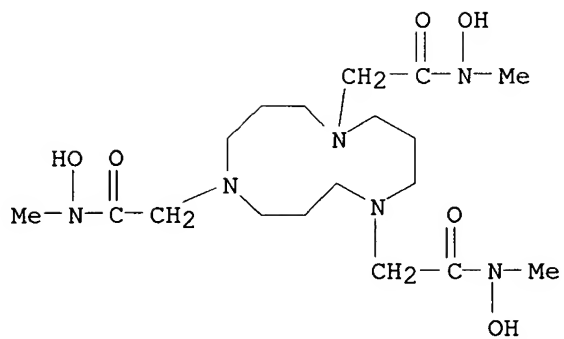
RN 169386-06-5 CAPLUS

CN 1,5,9-Triazacyclododecane-1,5,9-tricarboxamide, N,N',N''-trihydroxy-N,N',N''-trimethyl- (9CI) (CA INDEX NAME)



RN 247912-38-5 CAPLUS

CN 1,5,9-Triazacyclododecane-1,5,9-triacetamide, N,N',N''-trihydroxy-N,N',N''-trimethyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

130 ANSWER 30 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1999:429230 CAPLUS

DOCUMENT NUMBER: 131:199688

TITLE: Synthesis of new triazamacrocycles N-functionalized with α -(S)-hydroxycarboxylic acid pendant-arms

AUTHOR(S): Delagrangé, Samuel; Nepveu, Françoise

CORPORATE SOURCE: Laboratoire de Synthèse, Physico-Chimie et Radiobiologie, Université Paul Sabatier, Toulouse, 31062, Fr.

SOURCE: Tetrahedron Letters (1999), 40(27), 4989-4992

CODEN: TELEAY; ISSN: 0040-4039

PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The synthesis of two new macrocyclic ligands, N,N',N''-tris[2(S)-hydroxybutyric acid]-1,4,7-triazacyclononane [i.e., (S,S,S)-hexahydro- α,α',α'' -trihydroxy-1H-1,4,7-triazonine-1,4,7-tributanoic acid] and N,N',N''-tris[2(S)-hydroxybutyric acid]-1,5,9-triazacyclododecane [i.e., (S,S,S)-hexahydro- α,α',α'' -trihydroxy-1,5,9-triazacyclododecane-1,5,9-tributanoic acid] was reported. Each macrocycle bears three L-lactate-like pendant arms. Starting from L-malic acid, the absolute configuration of the α -(S)-hydroxy acid was kept along the synthesis leading to pure (S,S,S) enantiomers.

IT 241486-66-8P

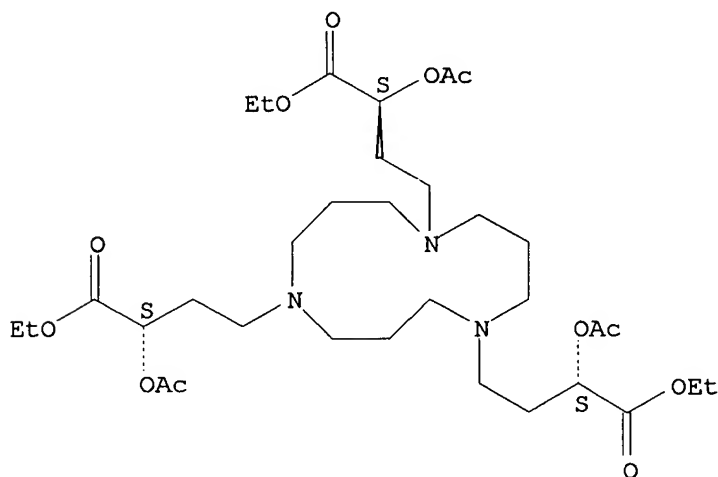
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of trihydroxytriazoninetricbutyrate and trihydroxytriazacyclododecanetricbutyrate)

RN 241486-66-8 CAPLUS

CN 1,5,9-Triazacyclododecane-1,5,9-tributanoic acid, α,α',α'' -tris(acetyloxy)-, triethyl ester, (α S, α' S, α'' S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



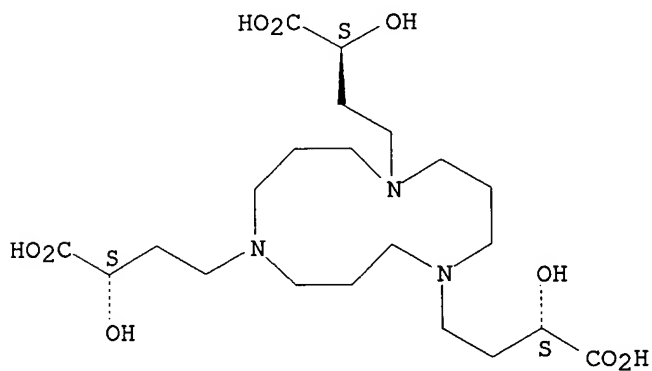
IT 241486-68-0P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of trihydroxytriazoninetricbutyrate and

10/680,076

trihydroxytriazacyclododecanetributyrate)
RN 241486-68-0 CAPLUS
CN 1,5,9-Triazacyclododecane-1,5,9-tributanoic acid,
 α,α',α'' -trihydroxy-, ($\alpha S,\alpha' S,\alpha'' S$)-
(9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT:

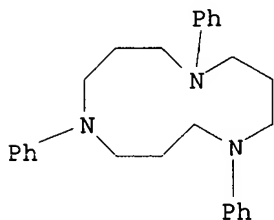
9

THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

~~130~~ ANSWER 31 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN
 X ACCESSION NUMBER: 1999:420940 CAPLUS
 DOCUMENT NUMBER: 131:74106
 TITLE: Catalyst for olefin polymerization
 INVENTOR(S): Sakai, Tatsuya
 PATENT ASSIGNEE(S): JSR Co., Ltd., Japan
 SOURCE: Jpn. Kokai Tokkyo Koho, 25 pp.
 CODEN: JKXXAF
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 11181013	A2	19990706	JP 1997-366004	19971224
PRIORITY APPLN. INFO.:			JP 1997-366004	19971224
OTHER SOURCE(S): MARPAT 131:74106				

AB Title catalyst for homopolymn. and copolymn. of polar olefins or cycloolefins comprises (I) a transition metal (vanadium, niobium, tantalum, molybdenum, tungsten, manganese, iron, cobalt, nickel, ruthenium, rhodium, palladium, iridium or platinum) coordinated with a cyclic compound having ≥ 2 nitrogen atoms in saturated bonds with carbon atoms, (II) an organo-aluminum compound (R1)aALZ3-a, wherein R1 is C1-20 hydrocarbon, Z is H, halogen, or alkoxy, $0 < a \leq 3$, and (III) an ionic compound. Thus, 1-hexene and ethylene were polymerized in the presence of methylaluminumoxane and 1,5,9-triazadodecanyl tantalum dichloride synthesized from 1,5,9-triazadodecane and tantalum pentachloride to give a copolymer with mol. weight 90,000, mol. weight distribution 2.52, and hexene content 31%.
 IT 228997-91-9
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (catalyst for olefin polymerization)
 RN 228997-91-9 CAPLUS
 CN 1,5,9-Triazacyclododecane, 1,5,9-triphenyl- (9CI) (CA INDEX NAME)



~~130~~ ANSWER 32 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1999:411134 CAPLUS

DOCUMENT NUMBER: 131:138432

TITLE: Synthesis, crystal structure and magnetic properties of a new dicopper(II) complex with a bis(macrocyclic) ligand

AUTHOR(S): Bu, Xian-He; Chen, Wei; Zhang, Ruo-Hua; Chen, Rong-Ti

CORPORATE SOURCE: Dep. Chem., Nankai Univ., Tianjin, 300071, Taiwan

SOURCE: Huaxue Xuebao (1999), 57(6), 627-634

CODEN: HHHPA4; ISSN: 0567-7351

PUBLISHER: Kexue Chubanshe

DOCUMENT TYPE: Journal

LANGUAGE: Chinese

AB A new binuclear Cu(II) complex, $[\text{Cu}_2\text{L}.\text{Br}_2]\text{Br} \cdot \text{H}_2\text{O}$, where L is a new binucleating macrocyclic ligand 2,6-bis(1,5,9-triazacyclododecan-9-ylmethyl)benzoate, was prepared and characterized by x-ray crystallog. Crystal data: monoclinic, space group $P2_1/c$, a 1.1666(2), b 1.3541(3), c 2.2750(5) nm, β 99.38(3)°, Z = 4. The binuclear Cu(II) center ions are bridged by a μ -carboxyl group of L and separated by 0.5884 nm. Both of the Cu(II) ion centers are coordinated by three amine nitrogens of [12]aneN3 subunit and one O of the carboxyl group, as well as one bromide ion. The Cu(II) ion is in the trigonal bipyramid environment. Variable temperature magnetic susceptibility studies indicate that there exists intramol.

antiferromagnetic coupling ($J = -22.49\text{cm}^{-1}$) between the two Cu(II) centers.

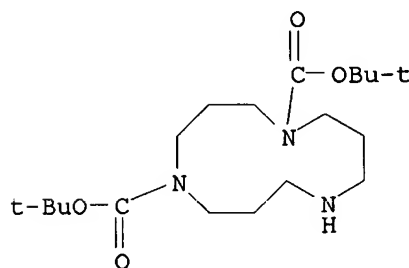
IT 174192-40-6

RL: RCT (Reactant); RACT (Reactant or reagent)

(for preparation of copper bis(triazacyclododecan-ylmethyl)benzoate dinuclear complex)

RN 174192-40-6 CAPLUS

CN 1,5,9-Triazacyclododecane-1,5-dicarboxylic acid, bis(1,1-dimethylethyl) ester (9CI) (CA INDEX NAME)



L30 ANSWER 33 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1999:357902 CAPLUS

DOCUMENT NUMBER: 131:214628

TITLE: Efficient syntheses of polymerizable pendant arm
azamacrocycles and formation of
poly(vinylbenzyltriazacyclododecane)AUTHOR(S): Long, Nicholas J.; Parker, David G.; Speyer, Paul R.;
White, Andrew J. P.; Williams, David J.CORPORATE SOURCE: Department of Chemistry, Imperial College of Science,
Technology and Medicine, South Kensington, London, SW7
2AY, UKSOURCE: Journal of the Chemical Society, Perkin Transactions
1: Organic and Bio-Organic Chemistry (1999), (12),
1621-1624

CODEN: JCPRB4; ISSN: 0300-922X

PUBLISHER: Royal Society of Chemistry

DOCUMENT TYPE: Journal

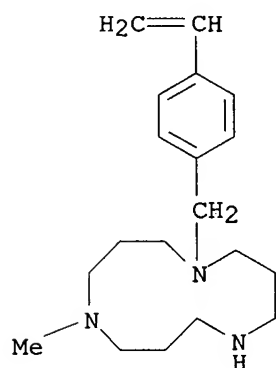
LANGUAGE: English

AB Synthetic routes to a number of metal-free triazacyclododecane derivs.
featuring the unsym. incorporation of polymerizable pendant side arms such
as vinylbenzene and methacrylate were developed. The structure of a
nitrate salt of the vinylbenzene-substituted species was determined by single
crystal X-ray diffraction and the first polymer-bound triazamacrocycles
formed via free-radical polymerization of a metal-free macrocycle-containing
monomer.

IT 243670-33-9P 243670-34-0P 243670-35-1P

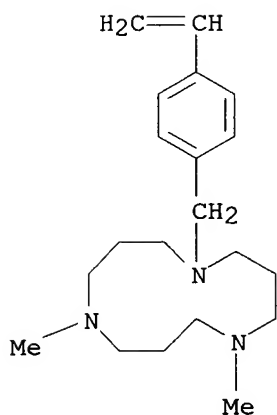
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP
(Preparation); RACT (Reactant or reagent)(efficient syntheses of polymerizable pendant arm azamacrocycles and
formation of poly(vinylbenzyltriazacyclododecane))

RN 243670-33-9 CAPLUS

CN 1,5,9-Triazacyclododecane, 1-[(4-ethenylphenyl)methyl]-5-methyl- (9CI)
(CA INDEX NAME)

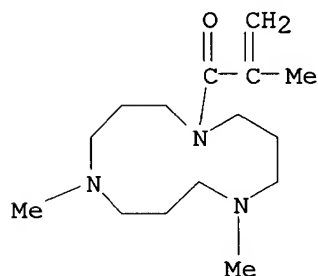
RN 243670-34-0 CAPLUS

CN 1,5,9-Triazacyclododecane, 1-[(4-ethenylphenyl)methyl]-5,9-dimethyl- (9CI)
(CA INDEX NAME)



RN 243670-35-1 CAPLUS

CN 1,5,9-Triazacyclododecane, 1,5-dimethyl-9-(2-methyl-1-oxo-2-propenyl)-
(9CI) (CA INDEX NAME)



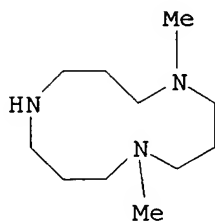
IT 139258-69-8

RL: RCT (Reactant); RACT (Reactant or reagent)

(efficient syntheses of polymerizable pendant arm azamacrocycles and
formation of poly(vinylbenzyltriazacyclododecane))

RN 139258-69-8 CAPLUS

CN 1,5,9-Triazacyclododecane, 1,5-dimethyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT:

26

THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

~~130~~ ANSWER 34 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1998:757792 CAPLUS

DOCUMENT NUMBER: 130:153220

TITLE: Palladium(0)-catalyzed allylation of highly acidic and non-nucleophilic arenesulfonamides, sulfamide, and cyanamide.II. Formation of medium and large heterocycles

AUTHOR(S): Cerezo, Silvia; Cortes, Jordi; Lopez-Romero, Juan-Manuel; Moreno-Manas, Marcial; Parella, Teodor; Pleixats, Roser; Roglans, Anna

CORPORATE SOURCE: Department of Chemistry, Universitat Autònoma de Barcelona, Barcelona, 08193, Spain

SOURCE: Tetrahedron (1998), 54(49), 14885-14904

CODEN: TETRAB; ISSN: 0040-4020

PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 130:153220

AB Arenesulfonamides, cyanamide derivs., and sulfamide derivs. react with allylic bis(carbonates) under Pd(0)-catalysis to afford medium and large unsatd. heterocycles instead of three and/or five-membered ring compds. Stable 15-membered palladium-containing rings were also isolated from arenesulfonamides with three trans olefinic systems coordinated to the metal. NMR and MALDI-TOF MS expts. were used for structure elucidation. Suitable hydrogenation conditions to give the saturated macrocycles were found.

IT 130927-35-4P 219839-43-7P 219839-47-1P

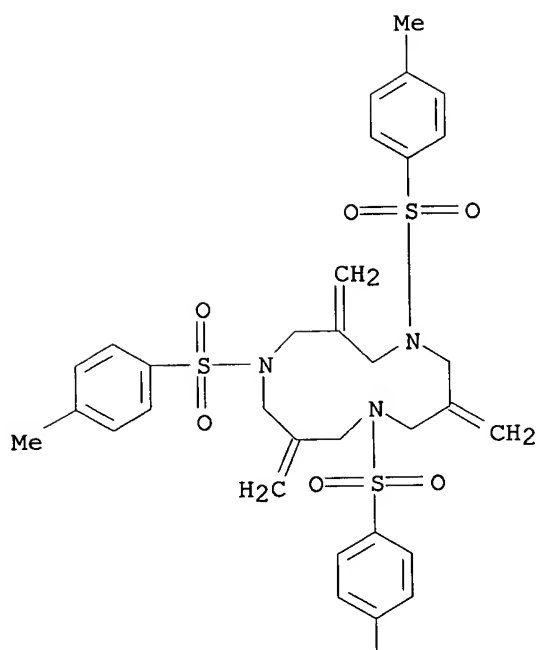
219839-49-3P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 130927-35-4 CAPLUS

CN 1,5,9-Triazacyclododecane, 3,7,11-tris(methylene)-1,5,9-tris[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)

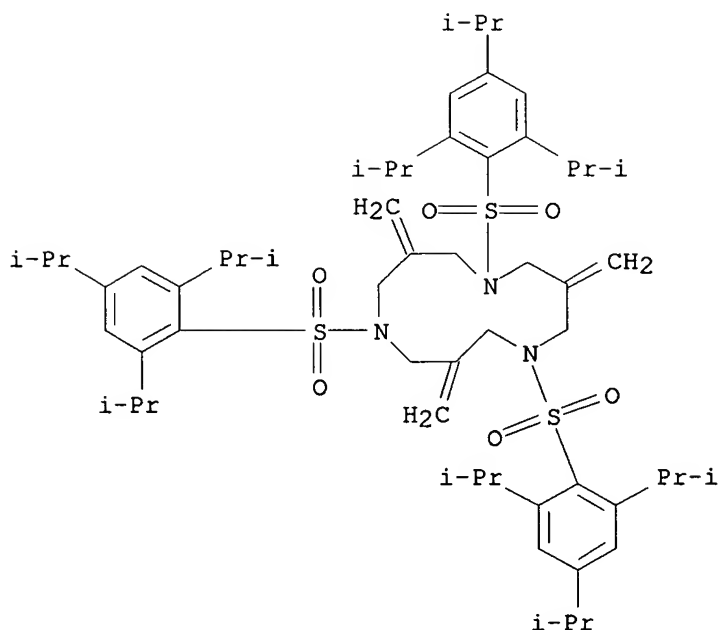
PAGE 1-A



PAGE 2-A

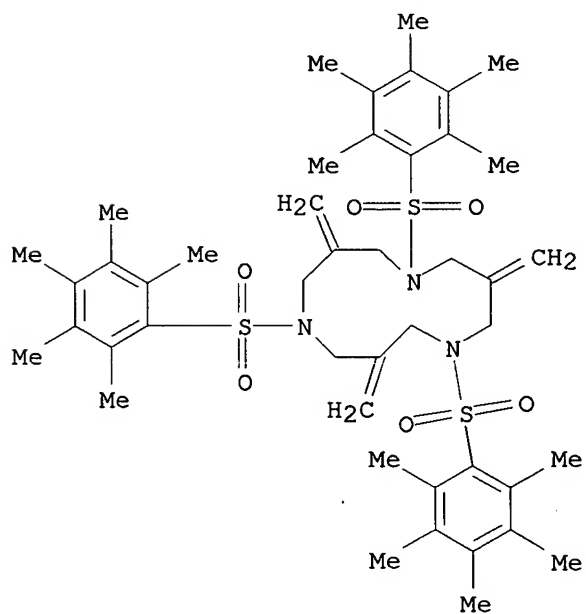


RN 219839-43-7 CAPLUS
 CN 1,5,9-Triazacyclododecane, 3,7,11-tris(methylene)-1,5,9-tris[[2,4,6-tris(1-methylethyl)phenyl]sulfonyl]- (9CI) (CA INDEX NAME)



RN 219839-47-1 CAPLUS

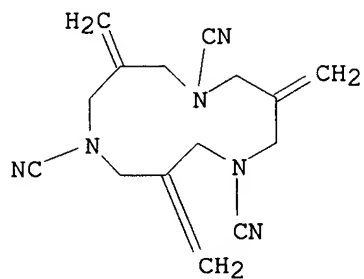
CN 1,5,9-Triazacyclododecane, 3,7,11-tris(methylene)-1,5,9-tris[(pentamethylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)



RN 219839-49-3 CAPLUS

CN 1,5,9-Triazacyclododecane-1,5,9-tricarbonitrile, 3,7,11-tris(methylene)- (9CI) (CA INDEX NAME)

10/680,076



REFERENCE COUNT:

42

THERE ARE 42 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

180 ANSWER 35 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1998:605672 CAPLUS

DOCUMENT NUMBER: 129:290121

TITLE: Reactions of Dichloroperfluorocycloalkenes with Triazamacrocyclic Amines

AUTHOR(S): Gupta, O. D.; Chen, Jianguo; Kirchmeier, Robert L.; Shreeve, Jean'ne M.

CORPORATE SOURCE: Department of Chemistry, University of Idaho, Moscow, ID, 83844-2343, USA

SOURCE: Inorganic Chemistry (1998), 37(20), 5342-5345

CODEN: INOCAJ; ISSN: 0020-1669

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

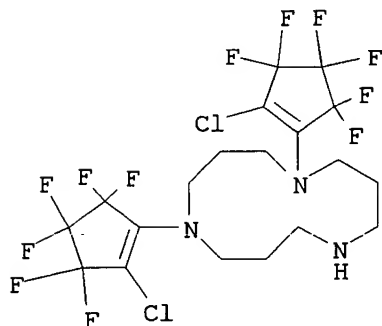
AB 1,2-Dichlorotetrafluorocyclobutene (A) and 1,2-dichlorohexafluorocyclopentene-1 (B) reacted with triazamacrocyclic amines 1,4,8-triazacycloundecane (1) and 1,5,9-triazacyclododecane (2) at 80° with stoichiometric amts. of NEt₃ in benzene. Cycloalkene A formed a 2:1 product 1,5-bis(chlorotetrafluorocyclobutenyl)-1,5,8-triazacycloundecane (3) with 1 and a 3:1 product 1,5,9-tris(chlorotetrafluorocyclobutenyl)-1,5,9-triazacyclododecane (4) with 2. B formed only 2:1 products 1,5-Bis(chlorohexafluorocyclopentenyl)-1,5,8-triazacycloundecane (5) and 1,5-Bis(chlorohexafluorocyclopentenyl)-1,5,9-triazacyclododecane (6) with 1 and 2, resp. The crystal structures of 3 and 4 were determined by single-crystal x-ray diffraction.

IT 214191-81-8P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation from reactions of dichloroperfluorocycloalkenes with triazamacrocyclic amines)

RN 214191-81-8 CAPLUS

CN 1,5,9-Triazacyclododecane, 1,5-bis(2-chloro-3,3,4,4,5,5-hexafluoro-1-cyclopenten-1-yl)- (9CI) (CA INDEX NAME)

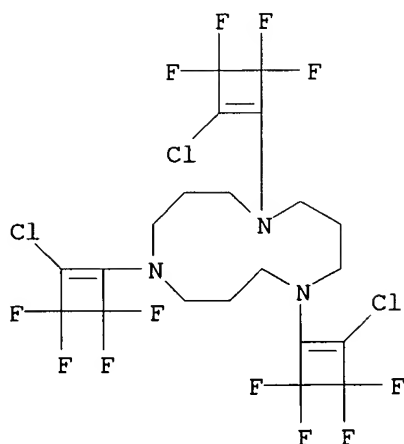


IT 214191-79-4P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation from reactions of dichloroperfluorocycloalkenes with triazamacrocyclic amines and crystal structure)

RN 214191-79-4 CAPLUS

CN 1,5,9-Triazacyclododecane, 1,5,9-tris(2-chloro-3,3,4,4-tetrafluoro-1-cyclobuten-1-yl)- (9CI) (CA INDEX NAME)



REFERENCE COUNT:

51

THERE ARE 51 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L30 ANSWER 36 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1998:263206 CAPLUS

DOCUMENT NUMBER: 128:266964

TITLE: Process of transfecting a cell with a polynucleotide mixed with an amphipathic compound and a DNA-binding protein

INVENTOR(S): Wolff, Jon A.; Fritz, Jeffery; Budker, Vladimir; Hagstrom, James

PATENT ASSIGNEE(S): Mirus Corporation, USA

SOURCE: U.S., 16 pp.

CODEN: USXXAM

DOCUMENT TYPE: Patent

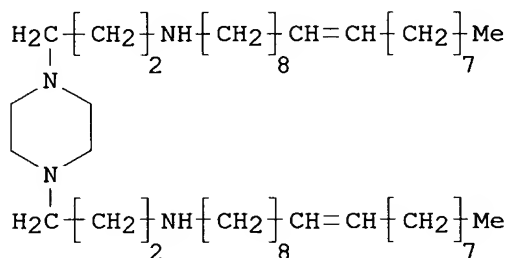
LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5744335	A	19980428	US 1995-530598	19950919
US 6180784	B1	20010130	US 1998-20566	19980117
PRIORITY APPLN. INFO.:			US 1995-530598	A3 19950919
OTHER SOURCE(S):	MARPAT	128:266964		

GI



AB Transfection of a cell is accomplished using with a polynucleotide mixed with one or more amphipathic compds. and a DNA-binding protein, especially a histone such as histones H1, H2A, or H2B. The DNA-binding protein may be fused to a nuclear localization signal peptide. Exemplary and preferred amphipathic compds. are cationic amphipathic compds. I was synthesized in 70% yield by reacting 1,4-bis(3-aminopropyl)piperazine with oleoyl chloride and reducing the intermediate with LiAlH₄ in THF. Histone H1 was found to increase the transfection efficiency of I 16.1-fold. I/H1 reagent has a greater transfection efficiency and less cellular toxicity than LipofectAmine, which is useful in gene therapy.

IT 205596-17-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

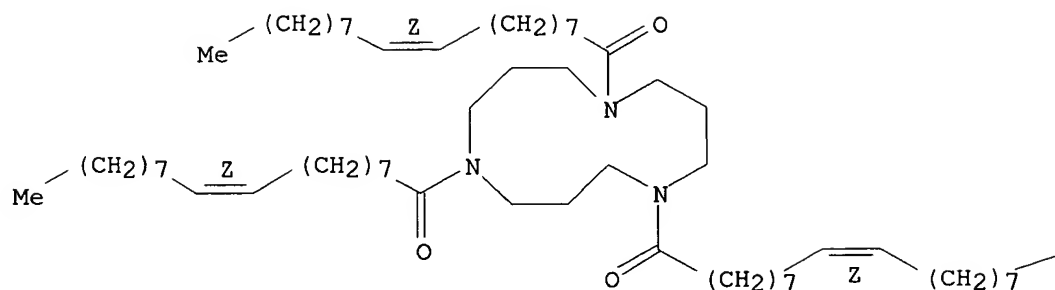
(amphipathic compds. for transfecting cells and their syntheses)

RN 205596-17-4 CAPLUS

CN 1,5,9-Triazacyclododecane, 1,5,9-tris(1-oxo-9-octadecenyl)-, (all-Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

PAGE 1-A



PAGE 1-B

Me

IT 205596-16-3P

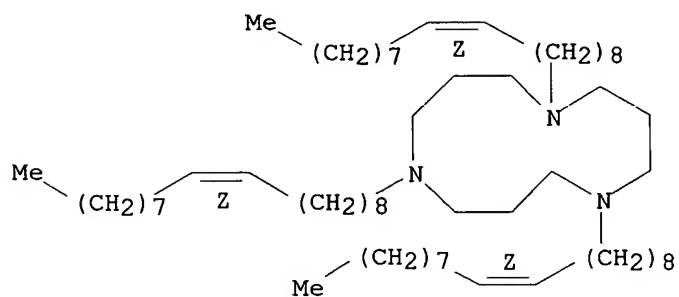
RL: BUU (Biological use, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(cell transfection with polynucleotide mixed with amphipathic compound and DNA-binding protein)

RN 205596-16-3 CAPLUS

CN 1,5,9-Triazacyclododecane, 1,5,9-tri-9-octadecenyl-, (all-Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



REFERENCE COUNT:

25

THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

~~L30~~ ANSWER 37 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1997:795802 CAPLUS

DOCUMENT NUMBER: 128:93621

TITLE: The azamacrocyclic derivatives of $H_4Ru_4(CO)_{12}$ and their reactivity with CO and catalytic activity in the methanol carbonylation and in the water-gas shift reaction

AUTHOR(S): Kallinen, K. O.; Pakkanen, T. T.; Pakkanen, T. A.

CORPORATE SOURCE: P.O. Box, University of Joensuu, Department of Chemistry, Joensuu FIN-80101, 111, Finland

SOURCE: Journal of Organometallic Chemistry (1997), 547(2), 319-327

CODEN: JORCAI; ISSN: 0022-328X

PUBLISHER: Elsevier Science S.A.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The reactions of $H_4Ru_4(CO)_{12}$ with cyclic triazaligands result in the formation of $[LH]+[H_3Ru_4(CO)_{12}]^-$ salts, (L=1,4,7-triazacyclononane, 1,4,7-trimethyl-1,4,7-triaza-cyclononane, 1,5,9-triazacyclododecane and 1,5,9-trimethyl-1,5,9-triazacyclo-dodecane). The compds. were synthesized by refluxing $H_4Ru_4(CO)_{12}$ in hexane followed by precipitation with the corresponding ligand. This is a convenient direct single-step synthetic route to produce $[H_3Ru_4(CO)_{12}]^-$ ion with a high yield. The compds. have been characterized by elemental anal. and spectroscopic measurements. In the 1H NMR spectra they showed a fluxional behavior. Reactivity towards CO at elevated temperature, and the catalytic activity of the new compds. in

the water-gas shift reaction (WGSR) and in the carbonylation of methanol, have been discussed.

IT 201154-76-9P

RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)

(azamacrocyclic derivs. of $H_4Ru_4(CO)_{12}$ and their reactivity with CO and catalytic activity in the methanol carbonylation and in the water-gas shift reaction)

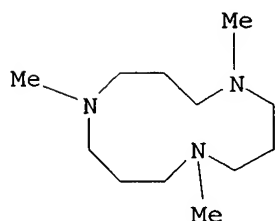
RN 201154-76-9 CAPLUS

CN Ruthenium, dodecacarbonyltetra- μ -hydrotetra-, tetrahedro, compd. with 1,5,9-trimethyl-1,5,9-triazacyclododecane (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 133256-59-4

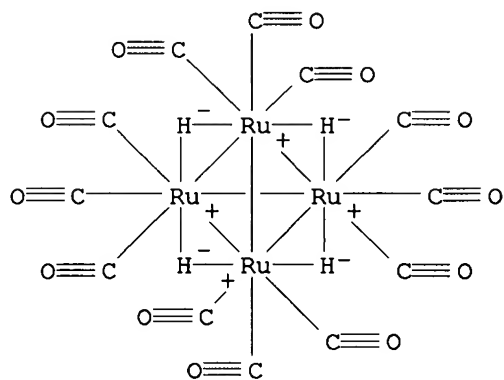
CMF C12 H27 N3



CM 2

10/680,076

CRN 34438-91-0
CMF C12 H4 O12 Ru4
CCI CCS



REFERENCE COUNT:

31

THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

130 ANSWER 38 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1997:753649 CAPLUS

DOCUMENT NUMBER: 128:121166

TITLE: Evaluation of solution structures of highly luminescent europium(III) chelates by using laser induced excitation of the 7F0→5D0 transition

AUTHOR(S): Latva, Martti; Takalo, Harri; Mikkala, Veli-Matti; Kankare, Jouko

CORPORATE SOURCE: Department of Chemistry, University of Turku, Turku, FIN-20014, Finland

SOURCE: Inorganica Chimica Acta (1998), 267(1), 63-72
CODEN: ICHAA3; ISSN: 0020-1693

PUBLISHER: Elsevier Science S.A.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Solution structures of 13 Eu(III) chelates were examined by using laser induced excitation of the 7F0→5D0 transition. Remarkable variations in the 7F0→5D0 excitation spectra of 2,2',2'',2'''-[[ary]bis(methylenenitrilo)]tetrakis(acetic acid) complexes of Eu(III) are observed depending on the denticity of the ligand and the number and character of the coordinated N atoms. The evaluation of the structures is made from the energy of the 7F0→5D0 excitation transition of Eu(III) because the 7F0→5D0 transition energy is dependent on the number and type of coordinating atoms in the 1st coordination sphere of Eu(III). Addnl. information about the structures is obtained by measuring the excited-state lifetimes of the Eu(III) chelates. The 7F0→5D0 transition energy shifts always an equal amount to lower energies due to the coordination of a certain group or atom. The energies of the 7F0→5D0 excitation transitions are also used to calculate these nephelauxetic shift parameters for coordinated N heteroatoms in the 2,2',2'',2'''-[[4-(phenylethynyl)pyridine-2,6-diyl]bis-(methylenenitrilo)]tetrakis(acetic acid) (3), 2,2',2'',2'''-[[2,2'-bipyridine-6,6'-diyl]bis-(methylenenitrilo)]tetrakis(acetic acid) (4), 2,2',2'',2'''-[[2,2':6'2''-terpyridine-6,6'-diyl]bis(methylenenitrilo)]tetrakis(acetic acid) (5), 2,2',2'',2'''-[[6,6'-(pyrazole-1,3-diyl)-bis(pyridine)-2,2'-diyl]bis(methylenenitrilo)]tetrakis(acetic acid) (7), 2,2',2'',2'''-[[6,6'-(thiazole-2,4-diyl)bis(pyridine)-2,2'-diyl]bis(methylenenitrilo)]tetrakis(acetic acid) (8) and 2,2',2'',2'''-[[2,2'-(pyridine-2,6-diyl)bis(thiazole)-4,4'-diyl]bis-(methylenenitrilo)]tetrakis(acetic acid) (9) complexes. The variation in the shift parameters of the N heteroatoms probably is due to the different distances between the N heteroatoms and Eu(III) ions.

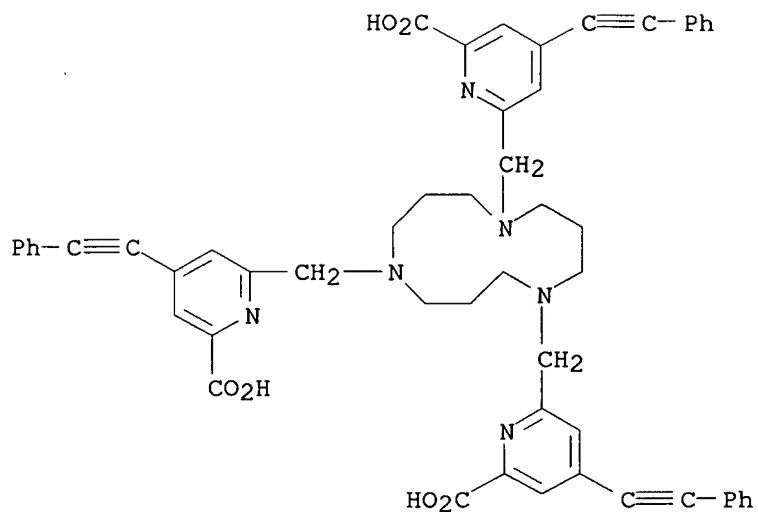
IT 201748-91-6D, europium complexes

RL: PRP (Properties)

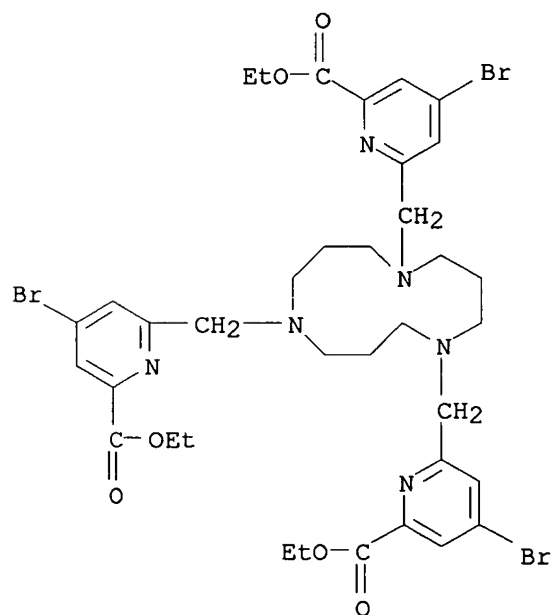
(evaluation of solution structures of highly luminescent europium(III) chelates by using laser induced excitation of 7F0→5D0 transition)

RN 201748-91-6 CAPLUS

CN 2-Pyridinecarboxylic acid, 6,6',6''-[1,5,9-triazacyclododecane-1,5,9-triyl]tris(methylene)]tris[4-(phenylethynyl)- (9CI) (CA INDEX NAME)

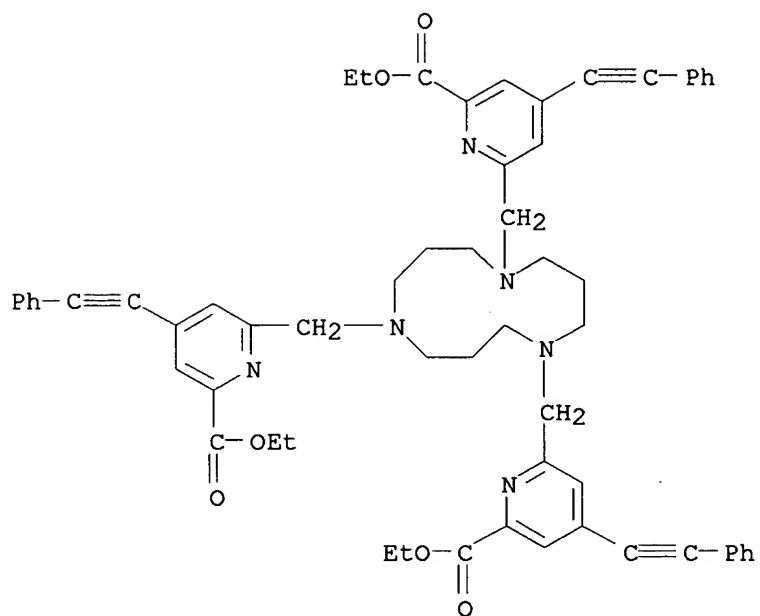


IT 201748-92-7P 201748-93-8P
 RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (evaluation of solution structures of highly luminescent europium(III) chelates by using laser induced excitation of 7F₀→5D₀ transition)
 RN 201748-92-7 CAPLUS
 CN 2-Pyridinecarboxylic acid, 6,6',6''-[1,5,9-triazacyclododecane-1,5,9-triyltris(methylene)]tris[4-bromo-, triethyl ester (9CI) (CA INDEX NAME)



RN 201748-93-8 CAPLUS
 CN 2-Pyridinecarboxylic acid, 6,6',6''-[1,5,9-triazacyclododecane-1,5,9-

triyltris(methylene)]tris[4-(phenylethynyl)-, triethyl ester (9CI) (CA
INDEX NAME)



REFERENCE COUNT:

45

THERE ARE 45 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

~~130~~ ANSWER 39 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1997:589536 CAPLUS

DOCUMENT NUMBER: 127:248091

TITLE: Synthesis and properties of N,N',N''-tris(1-naphthylmethyl)-1,5,9-triazacyclododecane

AUTHOR(S): Kubo, Kanji; Yamamoto, Emi; Sakurai, Tadamitsu

CORPORATE SOURCE: Department of Applied Chemistry, Faculty of Engineering, Kanagawa University, Yokohama, 221, Japan

SOURCE: Heterocycles (1997), 45(8), 1457-1461

CODEN: HTCYAM; ISSN: 0385-5414

PUBLISHER: Japan Institute of Heterocyclic Chemistry

DOCUMENT TYPE: Journal

LANGUAGE: English

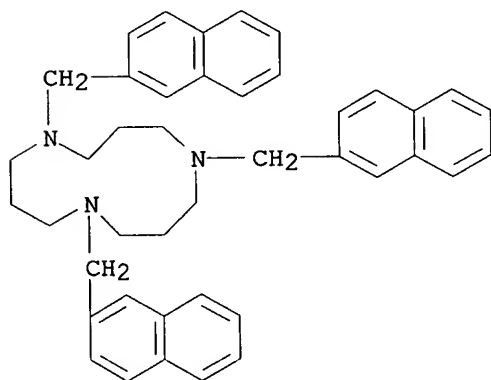
AB N,N'-Bis(1-naphthylmethyl)piperazine and N,N',N''-tris(1-naphthylmethyl)-1,5,9-triazacyclododecane were found to display unique photophys. properties for the guest salts. These guest salts enhanced the host emission remarkably by the inhibition of intramol. exciplex formation and then quenched the emission by photoinduced electron transfer from the counter anion to the naphthalene chromophore in the presence of high concns. of the salts.

IT 195883-54-6P

RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of tris(naphthylmethyl)triazacyclododecane and bis(naphthylmethyl)piperazine)

RN 195883-54-6 CAPLUS

CN 1,5,9-Triazacyclododecane, 1,5,9-tris(2-naphthalenylmethyl)- (9CI) (CA INDEX NAME)



REFERENCE COUNT:

21

THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

180 ANSWER 40 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1997:355708 CAPLUS

DOCUMENT NUMBER: 127:77654

TITLE: Iron release mechanism in a trihydroxamate siderophore analog. Kinetics and effect of pH

AUTHOR(S): Santos, M. A.; Bento, C.; Esteves, M. A.; Farinha, J. P. S.; Martinho, J. M. G.

CORPORATE SOURCE: Centro de Quimica Estrutural, Complexo I, Instituto Superior Tecnico, 1096, Lisbon, Port.

SOURCE: Inorganica Chimica Acta (1997), 258(1), 39-46

CODEN: ICHAA3; ISSN: 0020-1693

PUBLISHER: Elsevier

DOCUMENT TYPE: Journal

LANGUAGE: English

AB In view of the potential importance of the siderophore analog DOTRMAHA as an iron carrier in biol. systems, we have decided to study the mechanism and kinetics of iron release from the ferric DOTRMAHA complex to EDTA. The kinetics of the iron(III) exchange was monitored by UV-Vis absorption spectroscopy at the wavelength maximum of the iron(III) trihydroxamate complex. The decay of the complex absorbance with time is described as a sum of two exponentials plus a constant term. The mechanism of the exchange reaction is examined under conditions of varying concns. of the competing ligand and the hydrogen ion. The kinetics reveal pseudo-first order dependence of rate constant(s) on the EDTA concentration. Furthermore, pH dependence studies show that the exchange reaction is accelerated with increasing acidity of the medium. The results are mechanistically interpreted by a kinetic scheme involving two parallel pathways for the iron exchange: one is a bimol. process involving the direct attack of the EDTA on the ferric siderophore analog complex; the other involves initially the protonation of the complex followed by a rapid attack of the competing ligand. The set of kinetic data presented here is further rationalized in terms of known coordination and structural features of the DOTRMAHA ligand as well as the corresponding ferric complex, and compared with available data of some naturally occurring siderophores and synthetic analogs.

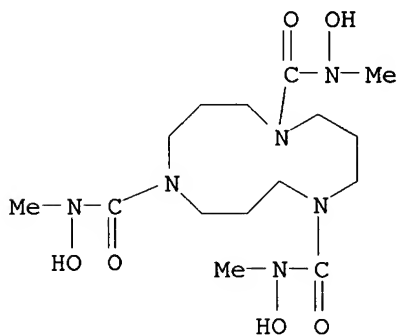
IT 169386-06-5, DOTRMAHA

RL: BSU (Biological study, unclassified); PEP (Physical, engineering or chemical process); BIOL (Biological study); PROC (Process)

(iron release mechanism in a trihydroxamate siderophore analog, kinetics and effect of pH)

RN 169386-06-5 CAPLUS

CN 1,5,9-Triazacyclododecane-1,5,9-tricarboxamide, N,N',N''-trihydroxy-N,N',N''-trimethyl- (9CI) (CA INDEX NAME)



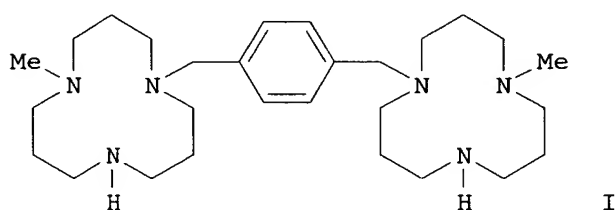
10/680,076

REFERENCE COUNT:

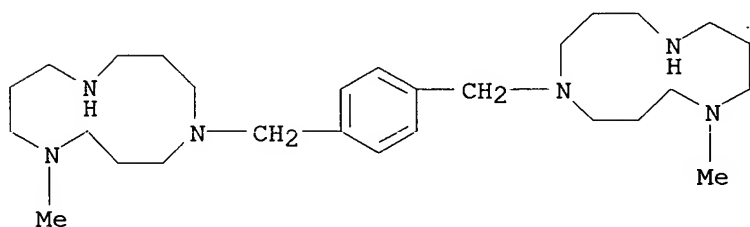
37

THERE ARE 37 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

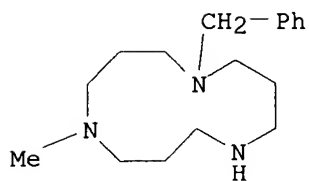
180 ANSWER 41 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN
 X ACCESSION NUMBER: 1997:190886 CAPLUS
 X DOCUMENT NUMBER: 126:293343
 TITLE: Synthesis and characterization of a new series of
 [12]aneN3 type macrocycles. Structures of two
 protonated metal-free ligands
 AUTHOR(S): Hubsch-Weber, Patricia; Youinou, Marie-Therese
 CORPORATE SOURCE: Lab. Chim. Metaux Transition Catalyse, Univ. Louis
 Pasteur, Strasbourg, 67000, Fr.
 SOURCE: Tetrahedron Letters (1997), 38(11), 1911-1914
 CODEN: TELEAY; ISSN: 0040-4039
 PUBLISHER: Elsevier
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI



AB The synthesis of a family of monotopic and ditopic ligands possessing a
 [12]aneN3 synthon and different spacers, e.g., I, is described. The
 characterization of two of them by x-ray diffraction is also reported.
 IT 189076-29-7P 189076-30-0P 189076-34-4P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of aneN3 macrocycles)
 RN 189076-29-7 CAPLUS
 CN 1,5,9-Triazacyclododecane, 1,1'-[1,4-phenylenebis(methylene)]bis[5-methyl-
 (9CI) (CA INDEX NAME)



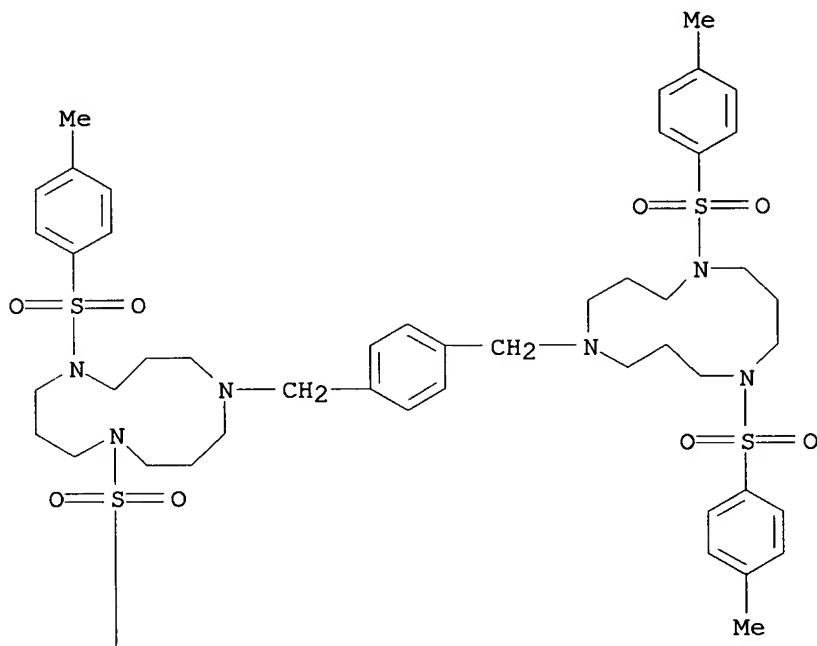
RN 189076-30-0 CAPLUS
 CN 1,5,9-Triazacyclododecane, 1-methyl-5-(phenylmethyl)- (9CI) (CA INDEX
 NAME)



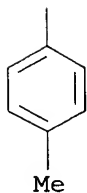
RN 189076-34-4 CAPLUS

CN 1,5,9-Triazacyclododecane, 1,1'-[1,4-phenylenebis(methylene)]bis[5,9-bis[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 2-A



REFERENCE COUNT:

21

THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

DB0 ANSWER 42 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1996:741489 CAPLUS

DOCUMENT NUMBER: 126:89764

TITLE: Macrocyclic triamines as linkers in two-armed receptors for peptides

AUTHOR(S): Iorio, Edward James; Still, W. Clark

CORPORATE SOURCE: Department Chemistry, Columbia University, New York, NY, 10027, USA

SOURCE: Bioorganic & Medicinal Chemistry Letters (1996), 6(22), 2673-2676

CODEN: BMCLE8; ISSN: 0960-894X

PUBLISHER: Elsevier

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Com. available triazamacrocycles have been substituted with trimesic acid/1,2-diamine cyclooligomers to create a new class of sequence-selective receptors for peptides. Screening of these compds. against a 3375-member library of N-acetyl tripeptides revealed novel peptide-binding properties.

IT 185756-45-0P

RL: BPR (Biological process); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); PROC (Process)

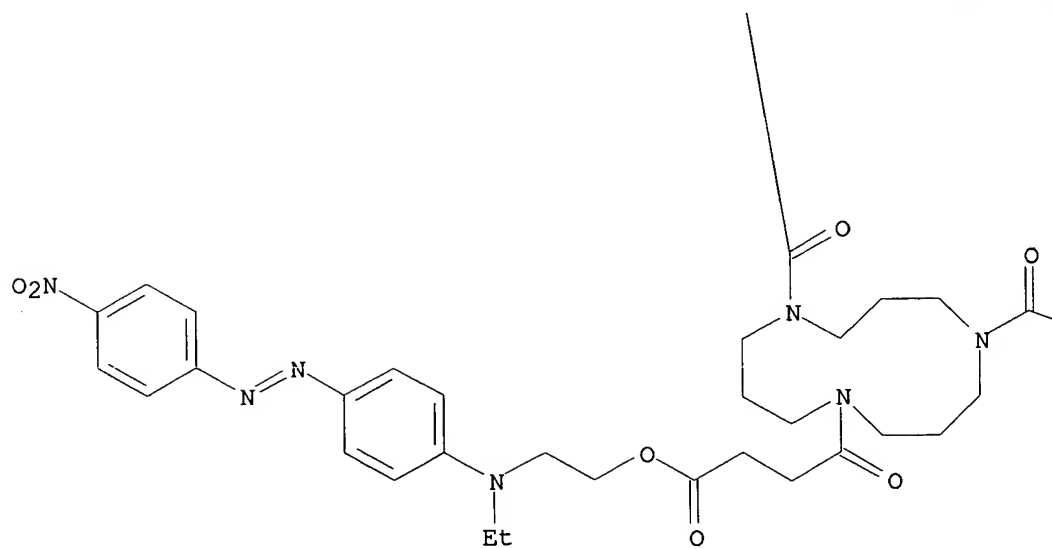
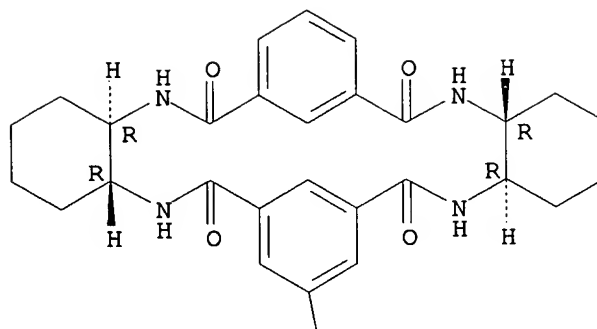
(preparation of macrocyclic triamines as linkers in two-armed receptors for peptides)

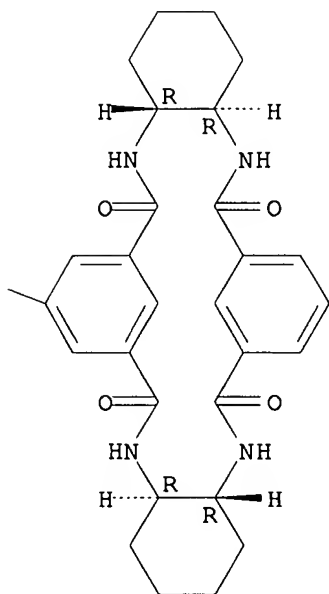
RN 185756-45-0 CAPLUS

CN 1,5,9-Triazacyclododecane-1-butanoic acid, 5,9-bis[(1,2,3,4,4a,5,6,12,13,13a,14,15,16,17,17a,18,19,25,26,26a-eicosahydro-6,12,19,25-tetraoxo-7,11:20,24-dimethenodibenzo[b,m][1,4,12,15]tetraazacyclodocosin-9-yl)carbonyl]-γ-oxo-, 2-[ethyl[4-[(4-nitrophenyl)azo]phenyl]amino]ethyl ester, [4aR-[4aR*,9(4aR*,13aR*,17aR*,26aR*),13aR*,17aR*,26aR*]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry unknown.





REFERENCE COUNT:

12

THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L30 ANSWER 43 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1996:635114 CAPLUS

DOCUMENT NUMBER: 125:265995

TITLE: Antiviral triaza compounds and their preparation

INVENTOR(S): Bell, Thomas W.

PATENT ASSIGNEE(S): Research Foundation of State University of New York, USA

SOURCE: PCT Int. Appl., 65 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

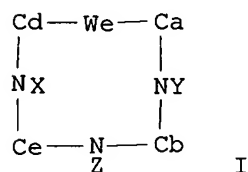
FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9625167	A1	19960822	WO 1996-US2132	19960216
W: AM, AT, AU, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LT, LU, LV, MD, MG, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, TJ, TM, TT				
RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
US 5663161	A	19970902	US 1995-392550	19950217
CA 2211920	AA	19960822	CA 1996-2211920	19960216
AU 9651704	A1	19960904	AU 1996-51704	19960216
AU 701783	B2	19990204		
EP 809504	A1	19971203	EP 1996-908473	19960216
EP 809504	B1	20020515		
R: AT, BE, CH, DE, DK, FR, GB, IT, LI, NL, SE, IE				
CN 1181013	A	19980506	CN 1996-193110	19960216
JP 11500130	T2	19990106	JP 1996-525169	19960216
AT 217529	E	20020615	AT 1996-908473	19960216
US 6342492	B1	20020129	US 1997-894491	19970807
PRIORITY APPLN. INFO.:			US 1995-392550	A2 19950217
			WO 1996-US2132	W 19960216

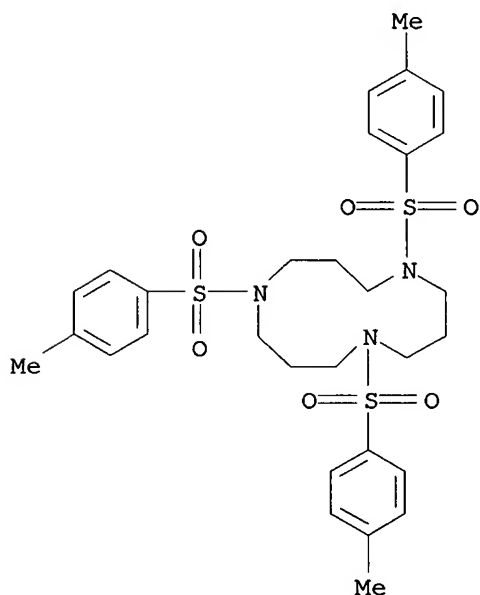
OTHER SOURCE(S): MARPAT 125:265995

GI

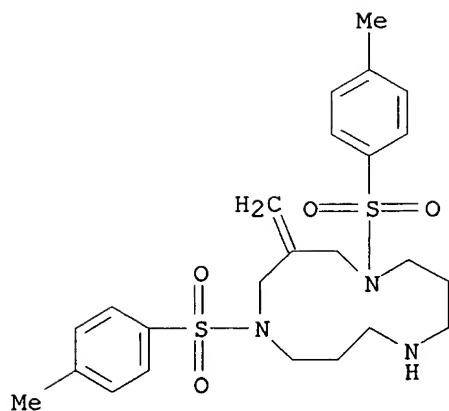


AB A method is disclosed for inhibiting viruses, in which a virus is contacted with an antiviral amount of I [W = bridge C with polar or nonpolar side group; X, Y = aromatic (aromatic = Ar (Ar = aromatic cyclic or aromatic heterocyclic ring of 5-7 members), Ar-sulfonyl, Ar-carboxy and Ar-alkyl), C1-10 alkyl, sulfonyl, carbonyl; Z = H, X, Y, C7-10 fused aryl; a, d, e = 0-10; b, c = 1-10]; the compds. are cyclic or acyclic and include sufficient Hydrogens for stable mols. Preparation of selected I is described, and activity against HIV and other viruses is presented.

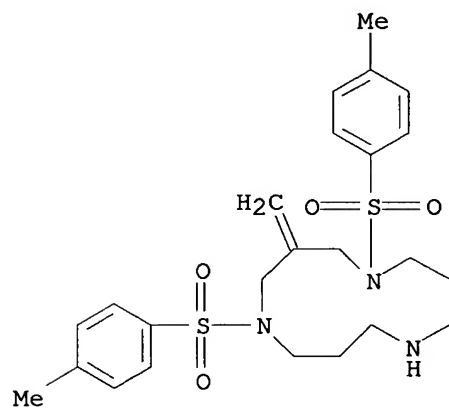
IT 35980-67-7P 182316-06-9DP, acyl derivative
 182316-06-9P 182316-08-1P 182316-10-5P
 182316-12-7P 182316-15-0P 182316-17-2P
 182316-19-4P 182316-20-7P 182316-21-8P
 182316-22-9P 182316-25-2P 182316-27-4DP, acyl
 derivative 182316-27-4P 182316-30-9P 182316-34-3P
 182316-44-5P 182316-50-3P
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological
 study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use);
 BIOL (Biological study); PREP (Preparation); USES (Uses)
 (antiviral triaza compound preparation and activity)
 RN 35980-67-7 CAPLUS
 CN 1,5,9-Triazacyclododecane, 1,5,9-tris[(4-methylphenyl)sulfonyl]- (9CI)
 (CA INDEX NAME)



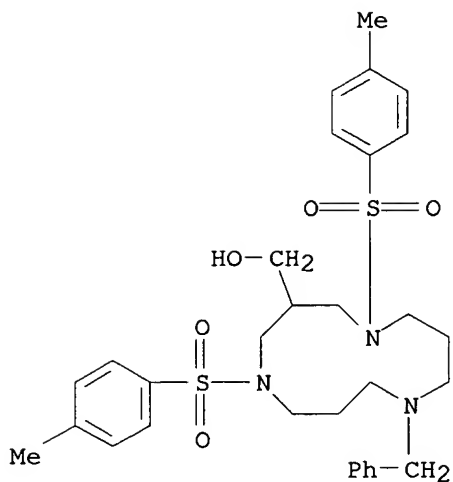
RN 182316-06-9 CAPLUS
 CN 1,5,9-Triazacyclododecane, 3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]-
 (9CI) (CA INDEX NAME)



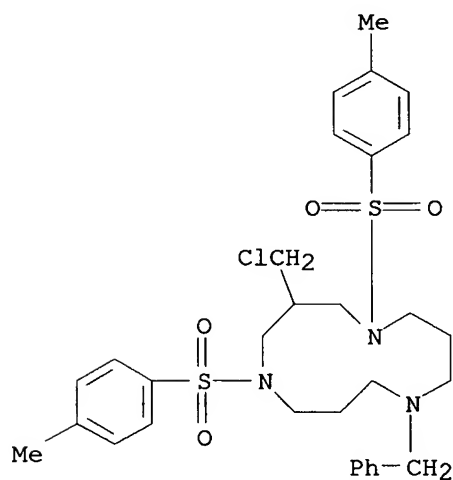
RN 182316-06-9 CAPLUS
 CN 1,5,9-Triazacyclododecane, 3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]-
 (9CI) (CA INDEX NAME)



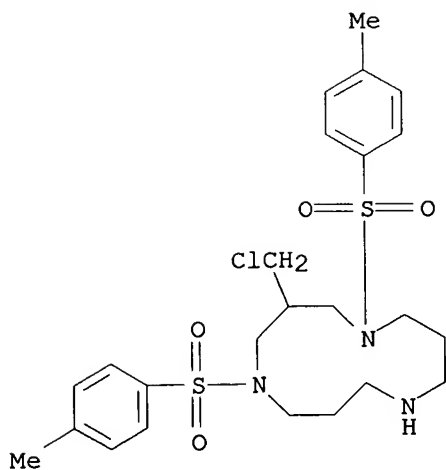
RN 182316-08-1 CAPLUS
 CN 1,5,9-Triazacyclododecane-3-methanol, 1,5-bis[(4-methylphenyl)sulfonyl]-9-
 (phenylmethyl)- (9CI) (CA INDEX NAME)



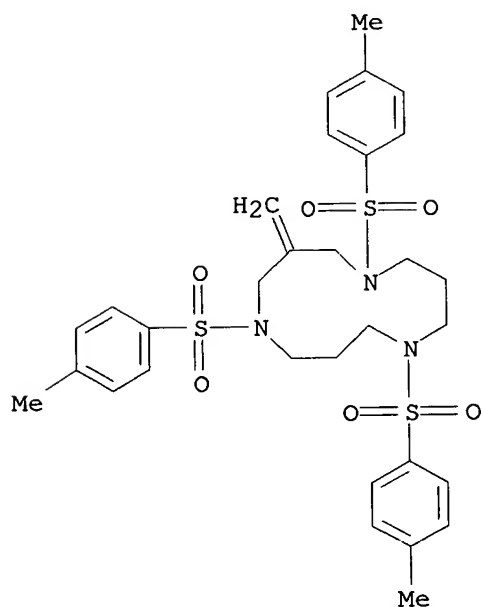
RN 182316-10-5 CAPLUS
 CN 1,5,9-Triazacyclododecane, 3-(chloromethyl)-1,5-bis[(4-methylphenyl)sulfonyl]-9-(phenylmethyl)- (9CI) (CA INDEX NAME)



RN 182316-12-7 CAPLUS
 CN 1,5,9-Triazacyclododecane, 3-(chloromethyl)-1,5-bis[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)

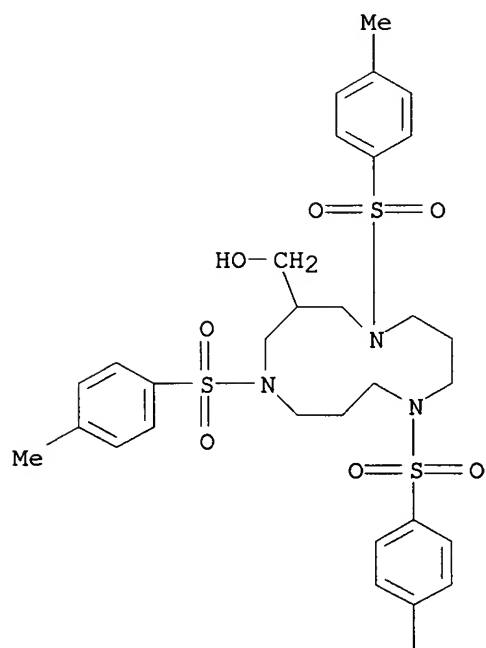


RN 182316-15-0 CAPLUS
 CN 1,5,9-Triazacyclododecane, 3-methylene-1,5,9-tris[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)



RN 182316-17-2 CAPLUS
 CN 1,5,9-Triazacyclododecane-3-methanol, 1,5,9-tris[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)

PAGE 1-A

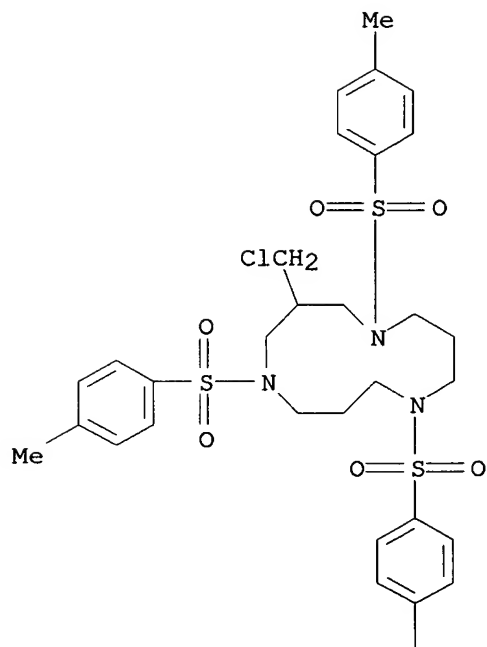


PAGE 2-A



RN 182316-19-4 CAPLUS
 CN 1,5,9-Triazacyclododecane, 3-(chloromethyl)-1,5,9-tris[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)

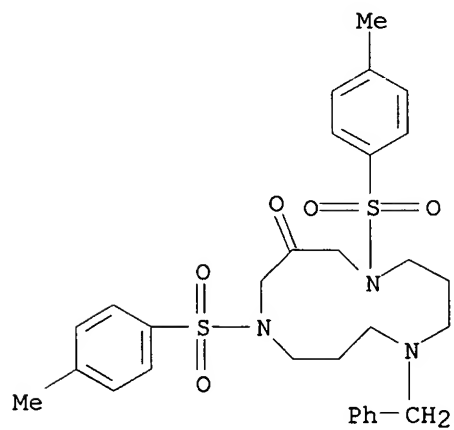
PAGE 1-A



PAGE 2-A

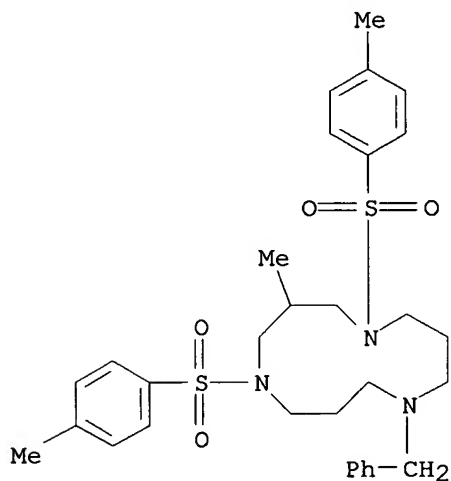


RN 182316-20-7 CAPLUS
 CN 1,5,9-Triazacyclododecan-3-one, 1,5-bis[(4-methylphenyl)sulfonyl]-9-(phenylmethyl)- (9CI) (CA INDEX NAME)



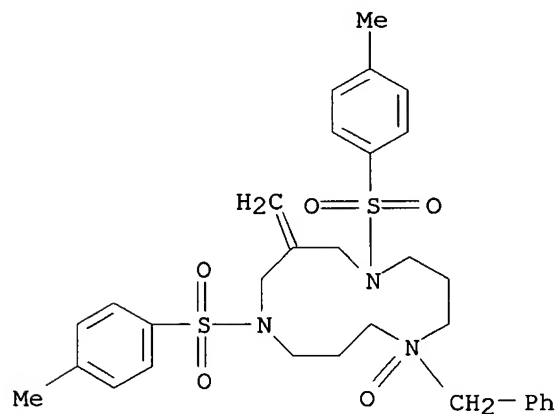
RN 182316-21-8 CAPLUS

CN 1,5,9-Triazacyclododecane, 3-methyl-1,5-bis[(4-methylphenyl)sulfonyl]-9-(phenylmethyl)- (9CI) (CA INDEX NAME)



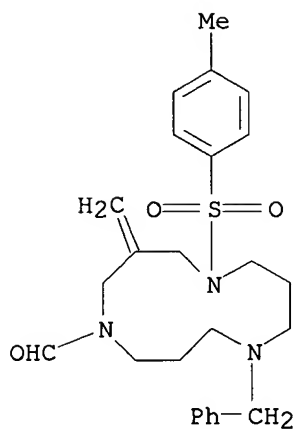
RN 182316-22-9 CAPLUS

CN 1,5,9-Triazacyclododecane, 3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]-9-(phenylmethyl)-, 9-oxide (9CI) (CA INDEX NAME)

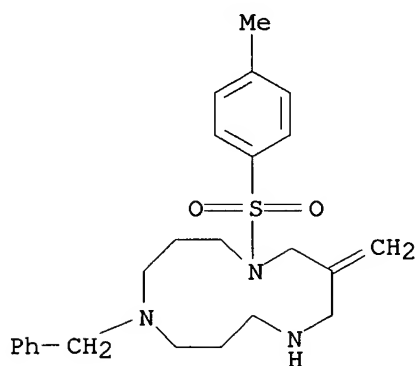


RN 182316-25-2 CAPLUS

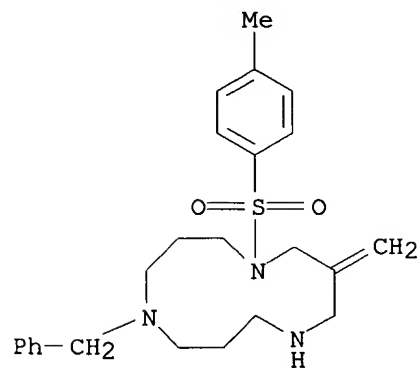
CN 1,5,9-Triazacyclododecane-1-carboxaldehyde, 3-methylene-5-[(4-methylphenyl)sulfonyl]-9-(phenylmethyl)- (9CI) (CA INDEX NAME)



RN 182316-27-4 CAPLUS
 CN 1,5,9-Triazacyclododecane, 3-methylene-1-[(4-methylphenyl)sulfonyl]-9-(phenylmethyl)- (9CI) (CA INDEX NAME)

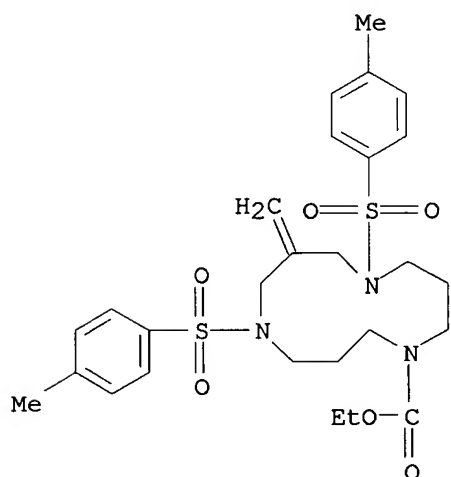


RN 182316-27-4 CAPLUS
 CN 1,5,9-Triazacyclododecane, 3-methylene-1-[(4-methylphenyl)sulfonyl]-9-(phenylmethyl)- (9CI) (CA INDEX NAME)



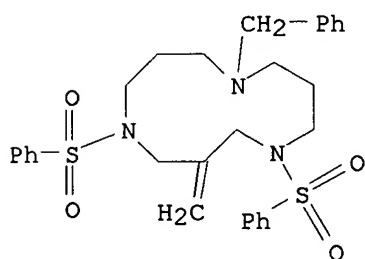
RN 182316-30-9 CAPLUS

CN 1,5,9-Triazacyclododecane-1-carboxylic acid, 7-methylene-5,9-bis[(4-methylphenyl)sulfonyl]-, ethyl ester (9CI) (CA INDEX NAME)



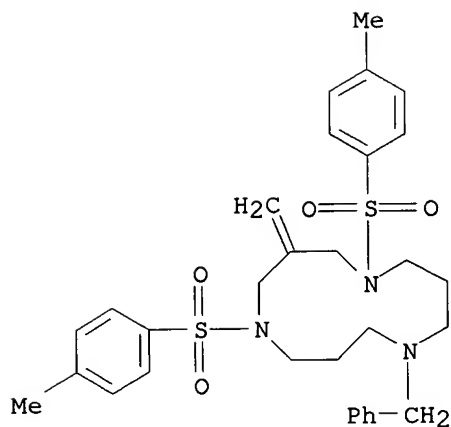
RN 182316-34-3 CAPLUS

CN 1,5,9-Triazacyclododecane, 3-methylene-9-(phenylmethyl)-1,5-bis(phenylsulfonyl)- (9CI) (CA INDEX NAME)

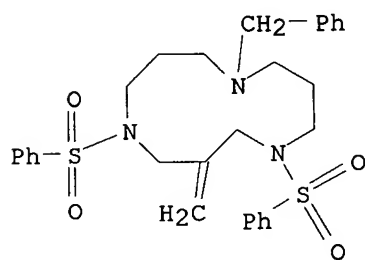


RN 182316-44-5 CAPLUS

CN 1,5,9-Triazacyclododecane, 3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]-9-(phenylmethyl)- (9CI) (CA INDEX NAME)



RN 182316-50-3 CAPLUS
 CN 1,5,9-Triazacyclododecane, 3-methylene-9-(phenylmethyl)-1,5-bis(phenylsulfonyl)-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

180 ANSWER 44 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1996:354980 CAPLUS

DOCUMENT NUMBER: 125:97175

TITLE: Complexation behavior of C- and N-functionalized
tetradentate ligands based on 1,5,9-
triazacyclododecane

AUTHOR(S): Bates, George B.; Parker, David

CORPORATE SOURCE: Dep. Chem., Univ. Durham, Durham, DH1 3LE, UK

SOURCE: Journal of the Chemical Society, Perkin Transactions

2: Physical Organic Chemistry (1996), (6), 1109-1115

CODEN: JCPKBH; ISSN: 0300-9580

PUBLISHER: Royal Society of Chemistry

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The synthesis and aqueous complexation behavior of C- and N-linked
o-hydroxyaryl substituted derivs. of 1,5,9-triazacyclododecane is
reported. The N-linked ligand forms strong 1:1 complexes with copper and
zinc (log KML = 18.7 and 14.1, resp.) in which the phenolate acts as an
effective donor ligand in the putative tetrahedral complex. The ligand
substituted at carbon at the 3-position is less basic and forms much
weaker complexes with Cu²⁺, Ni²⁺ and Zn²⁺ (log KCuL 10.2, log KZnL 7.32
and log KNiL 6.11) in which phenolate participation is absent.

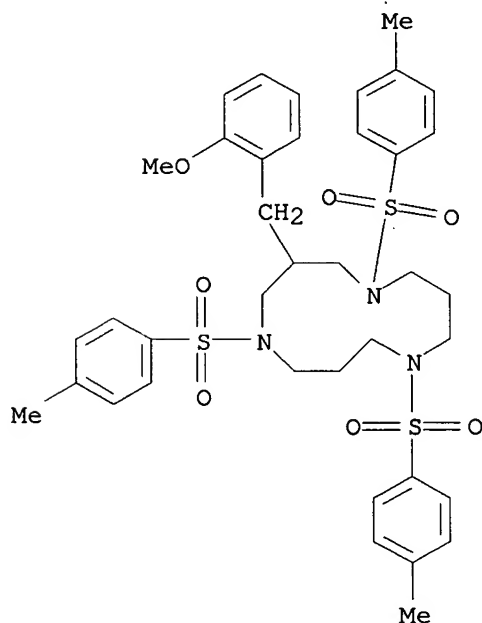
IT 178879-52-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)

(in preparation of hydroxybromobenzyl triazacyclododecane)

RN 178879-52-2 CAPLUS

CN 1,5,9-Triazacyclododecane, 3-[(2-methoxyphenyl)methyl]-1,5,9-tris[(4-
methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)



10/680,076

180 ANSWER 45 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1996:294877 CAPLUS

DOCUMENT NUMBER: 124:343341

TITLE: Preparation of cyclic polyamines as antiviral agents

INVENTOR(S): Iwata, Masaaki; Yamamoto, Naoki; Nakajima, Hideki

PATENT ASSIGNEE(S): Rikagaku Kenkyuzyo, Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 35 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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JP 08027129	A2	19960130	JP 1994-165028	19940718
PRIORITY APPLN. INFO.: GI			JP 1994-165028	19940718

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Cyclic polyazaalkanes, in which 3-20 C2, C3, or C4 alkylene chains and NH are alternately linked, are prepared. Thus, the title compound (I.8HBr) was prepared by condensation of 1,5,9-triazacyclododecane derivative (III; Ts = p-toluenesulfonyl) with 1,3-dibromopropane in the presence of NaHCO₃ at 70° for 4 days followed by detosylation. I.8HBr and another title compound (II.20HBr) showed ED₅₀ of 2.5 and 0.67 μ M for inhibiting the death of HIV-infected MT-4 cells (vs. 0.019 μ M for AZT) and 50% cytotoxic concentration of 470 and 8.6 μ M, resp., against MT-4 cells (vs. 247.25 μ M).

IT 164913-15-9P 164913-31-9P 164913-40-0P

167080-92-4P 167080-93-5P 167080-99-1P

176493-19-9P 176493-21-3P 176493-22-4P

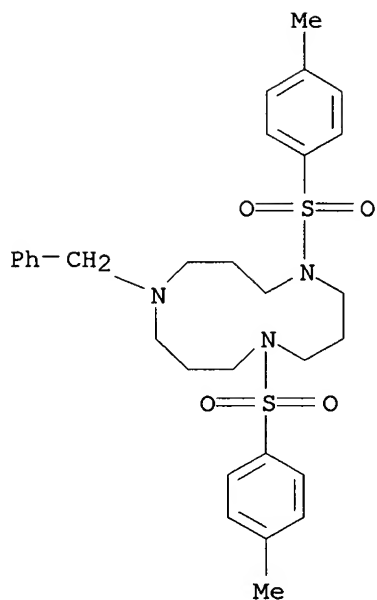
176493-23-5P 176493-25-7P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of cyclic polyazaalkanes as antiviral agents)

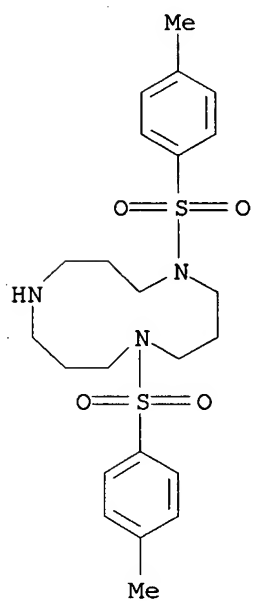
RN 164913-15-9 CAPLUS

CN 1,5,9-Triazacyclododecane, 1,5-bis[(4-methylphenyl)sulfonyl]-9-(phenylmethyl)-(9CI) (CA INDEX NAME)



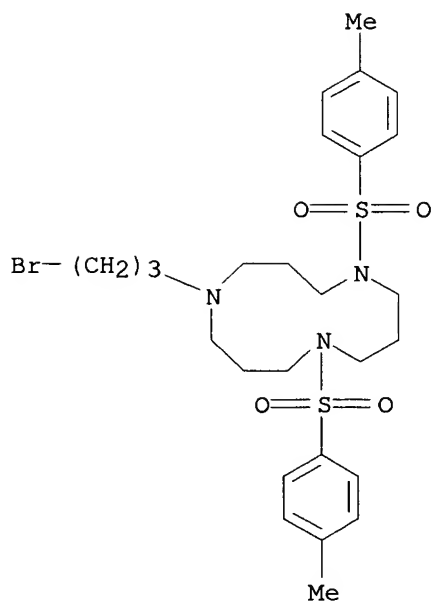
RN 164913-31-9 CAPLUS

CN 1,5,9-Triazacyclododecane, 1,5-bis[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)



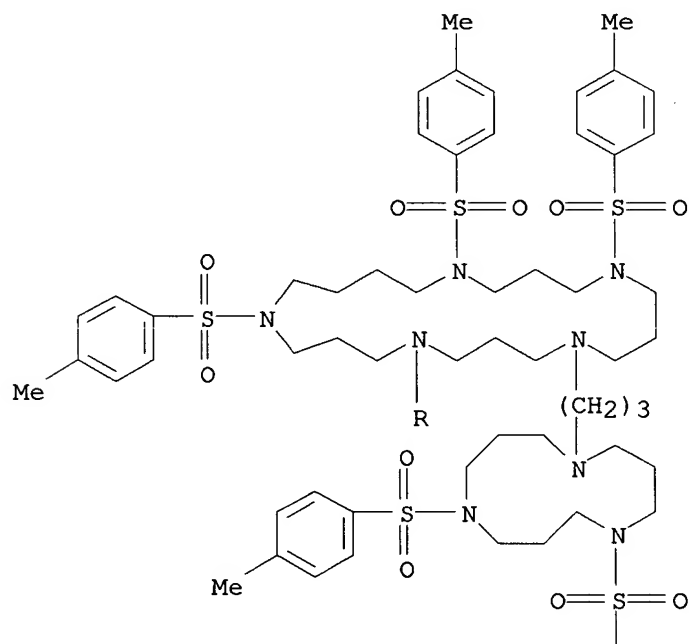
RN 164913-40-0 CAPLUS

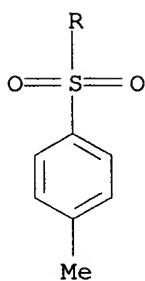
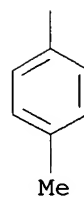
CN 1,5,9-Triazacyclododecane, 1-(3-bromopropyl)-5,9-bis[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)



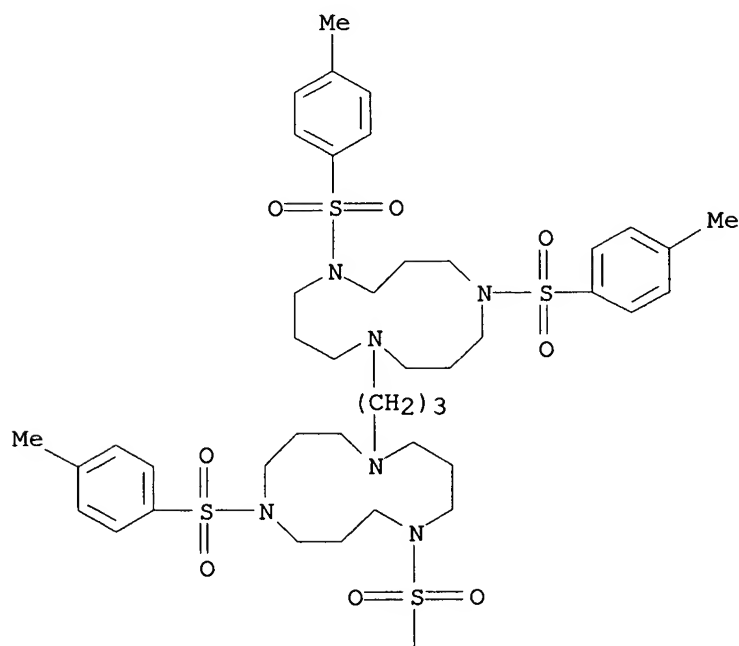
RN 167080-92-4 CAPLUS
 CN 1,5,9,13,17-Pentaazacyclododecane, 9-[3-[5,9-bis[(4-methylphenyl)sulfonyl]-1,5,9-triazacyclododec-1-yl]propyl]-1,5,13,17-tetrakis[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)

PAGE 1-A

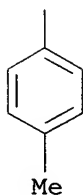




RN 167080-93-5 CAPLUS
 CN 1,5,9-Triazacyclododecane, 1,1'-(1,3-propanediyl)bis[5,9-bis[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)



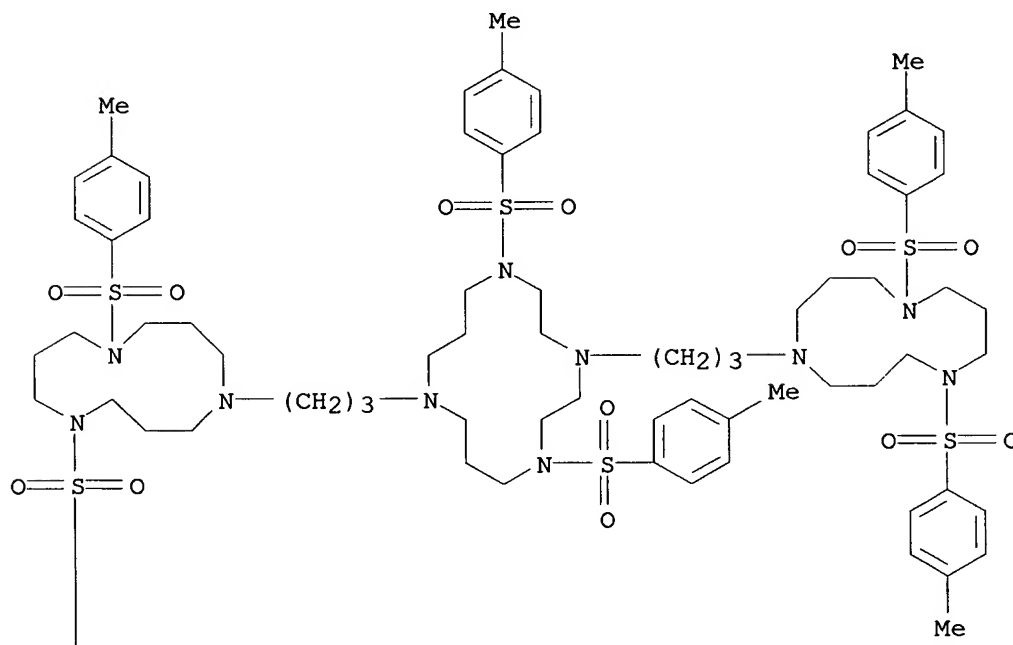
PAGE 2-A



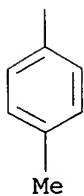
RN 176493-21-3 CAPLUS

CN 1,4,7,11-Tetraazacyclotetradecane, 4,11-bis[3-[5,9-bis[(4-methylphenyl)sulfonyl]-1,5,9-triazacyclododec-1-yl]propyl]-1,7-bis[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 2-A

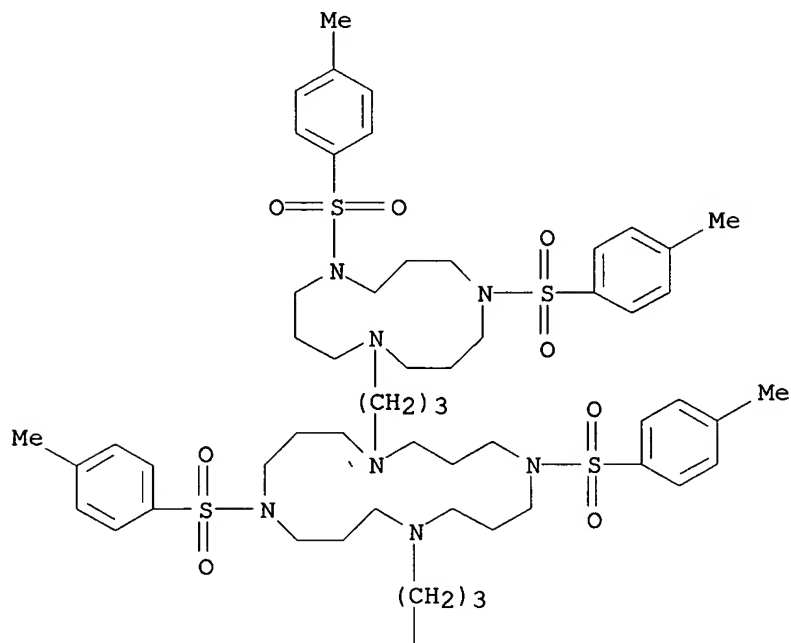


RN 176493-22-4 CAPLUS

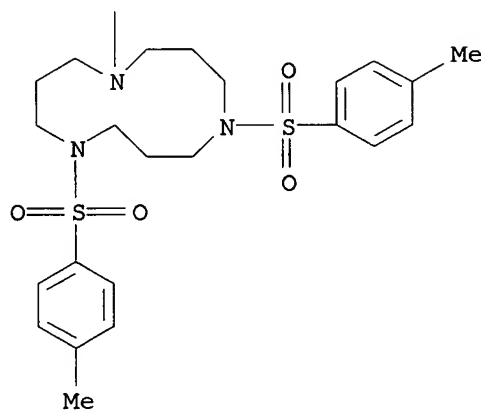
CN 1,5,9,13-Tetraazacyclohexadecane, 1,9-bis[3-[5,9-bis[(4-

methylphenyl) sulfonyl]-1,5,9-triazacyclododec-1-yl]propyl]-5,13-bis[(4-methylphenyl) sulfonyl]- (9CI) (CA INDEX NAME)

PAGE 1-A

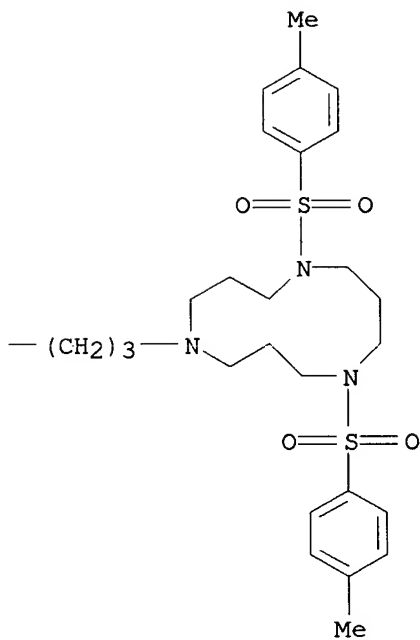
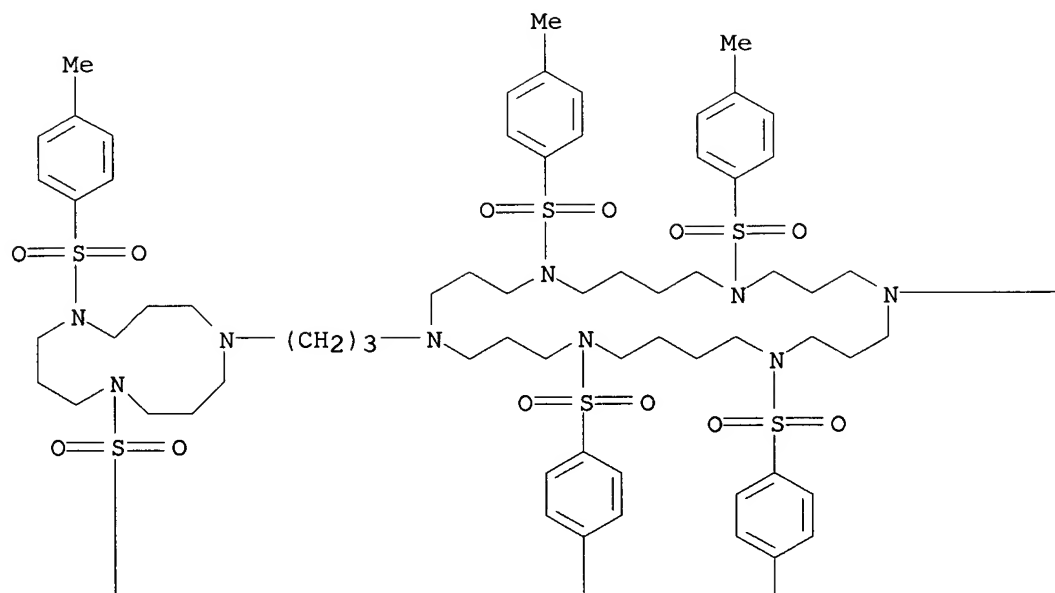


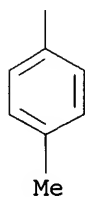
PAGE 2-A



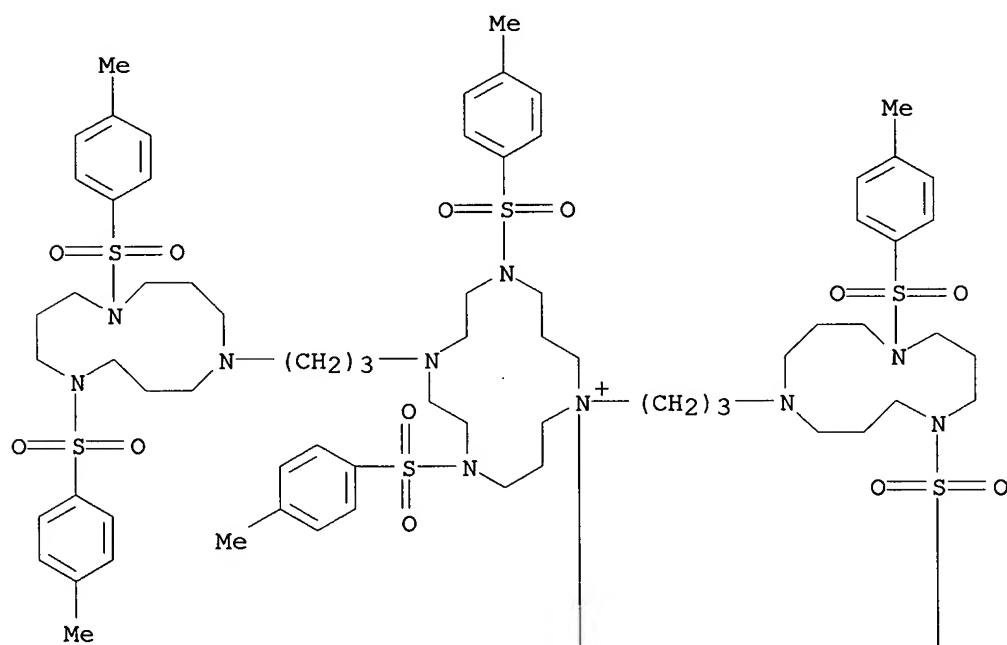
RN 176493-23-5 CAPLUS

CN 1,5,9,14,18,22-Hexaazacyclohexacosane, 5,18-bis[3-[5,9-bis[(4-methylphenyl) sulfonyl]-1,5,9-triazacyclododec-1-yl]propyl]-1,9,14,22-tetrakis[(4-methylphenyl) sulfonyl]- (9CI) (CA INDEX NAME)

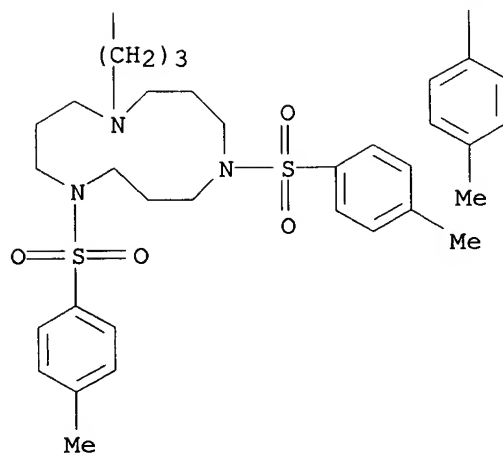




RN 176493-25-7 CAPLUS
 CN 1,4,7-Triaza-11-azoniacyclotetradecane, 4,11,11-tris[3-[5,9-bis[(4-methylphenyl)sulfonyl]-1,5,9-triazacyclododec-1-yl]propyl]-1,7-bis[(4-methylphenyl)sulfonyl]-, bromide (9CI) (CA INDEX NAME)



PAGE 2-A

● Br⁻

130 ANSWER 46 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1996:157892 CAPLUS

DOCUMENT NUMBER: 124:305467

TITLE: New facile and convenient synthesis of bispolyazamacrocycles using Boc protection. Determination of geometric parameters of dinuclear copper(II) complexes using ESR spectroscopy and molecular mechanics calculations

AUTHOR(S): Brandes, Stephane; Gros, Claude; Denat, Franck; Pullumbi, Pluton; Guillard, Roger

CORPORATE SOURCE: Lab. d'Ingenierie Moleculaire Separation applications Gaz, Univ. Bourgogne, Dijon, 21100, Fr.

SOURCE: Bulletin de la Societe Chimique de France (1996), 133(1), 65-73

CODEN: BSCFAS; ISSN: 0037-8968

PUBLISHER: Elsevier

DOCUMENT TYPE: Journal

LANGUAGE: English

AB A new facile and convenient synthetic route was designed for the preparation of bispolyazamacrocycles in high yields by direct condensation of the readily available intermediate N,N'-diboctriaazamacrocyclic or N,N',N''-tribocetraazamacrocycles with aromatic biselectrophiles, ie, o-, m-, p-xylyl and anthracenyl derivs. The use of a versatile group, such as tert-butyloxycarbonyl (Boc), which is easily removed within 1 h by treatment with 6 M HCl or TFA, leads to polyazamacrocycles in which one N is discriminated from the others. The anthracenyl and o-xylyl dimers were synthesized by reacting diacyl chloride to give the corresponding diamides. Further reduction of the amide groups and elimination of the protecting Boc moieties were carried in a 1-pot reaction with BH₃-THF followed by acid treatment. In parallel, exclusive mono-N-alkylation of the available secondary amine of the same protected macrocycle with the corresponding dibromoxylene gave the meta and para dimers; the protecting moieties were eliminated in a similar way. ESR measurements of spin-spin distances of the dicopper complexes were determined from the ratio of the intensity of the forbidden transition to the intensity of the allowed transitions. Mol. mechanics calcns. were also undertaken to evaluate the Cu-Cu distance by using a new rule-based force field.

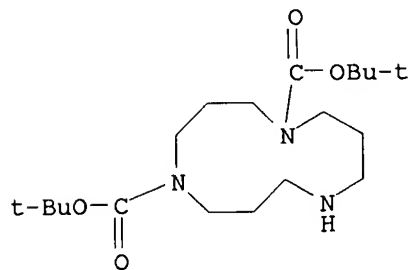
IT 174192-40-6P 175854-44-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(for preparation of bispolyazamacrocycles)

RN 174192-40-6 CAPLUS

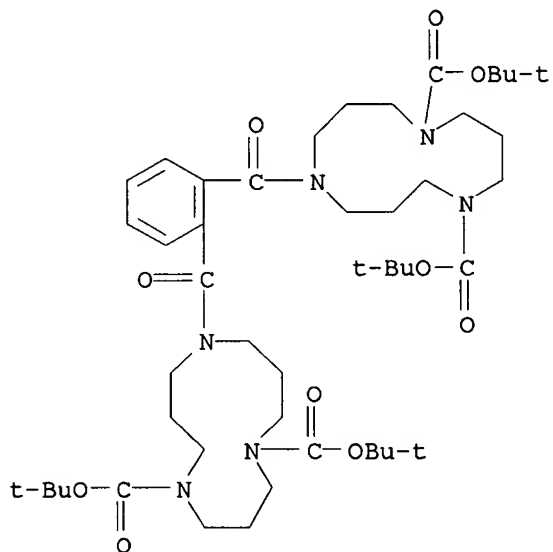
CN 1,5,9-Triazacyclododecane-1,5-dicarboxylic acid, bis(1,1-dimethylethyl) ester (9CI) (CA INDEX NAME)



10/680,076

RN 175854-44-1 CAPLUS

CN 1,5,9-Triazacyclododecane-1,5-dicarboxylic acid, 9,9'-(1,2-phenylenedicarbonyl)bis-, tetrakis(1,1-dimethylethyl) ester (9CI) (CA INDEX NAME)



130 ANSWER 47 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1996:113714 CAPLUS

DOCUMENT NUMBER: 124:202189

TITLE: Conversion of Macrocyclic Polyamines into Carbon-Substituted Derivatives. Synthesis of Derivatives of 1,5,9-Triazacyclododecane-2-carbonitrile

AUTHOR(S): Brunet, Philippe; Wuest, James D.

CORPORATE SOURCE: Departement de Chimie, Universite de Montreal, Montreal, QC, H3C 3J7, Can.

SOURCE: Journal of Organic Chemistry (1996), 61(5), 1847-9
CODEN: JOCEAH; ISSN: 0022-3263

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 124:202189

AB Diprotected derivs. of 1,5,9-triazacyclododecane were converted into diprotected derivs. of 1,5,9-triazacyclododecane-2-carbonitrile in good overall yield by oxidation with Na₂WO₄/H₂O₂, addition of KCN, and reduction with

TiCl₃. This strategy promises to be a useful general method for the direct conversion of macrocyclic polyamines into carbon-substituted derivs. that would otherwise not be readily available.

IT 164913-31-9P 174192-36-0P 174192-38-2P

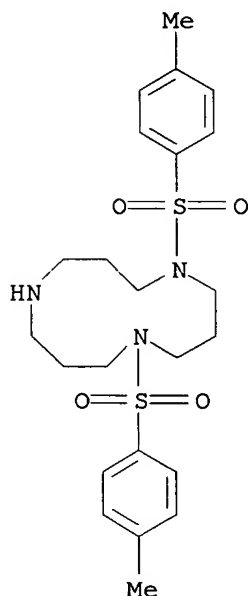
174192-39-3P 174192-40-6P 174192-41-7P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(regioselective oxidative cyanation method for macrocyclic polyamines)

RN 164913-31-9 CAPLUS

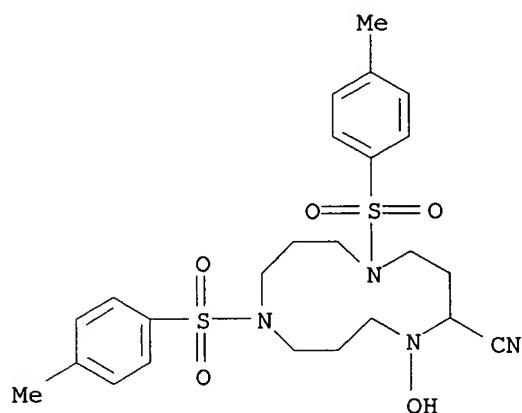
CN 1,5,9-Triazacyclododecane, 1,5-bis[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)



RN 174192-36-0 CAPLUS

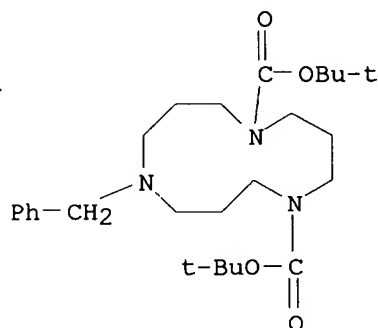
CN 1,5,9-Triazacyclododecane-2-carbonitrile, 1-hydroxy-5,9-bis[(4-

methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)



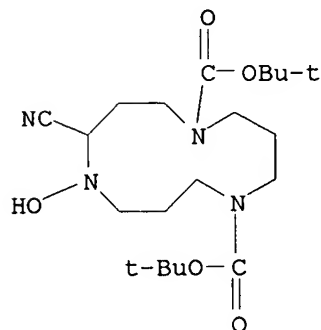
RN 174192-38-2 CAPLUS

CN 1,5,9-Triazacyclododecane-1,5-dicarboxylic acid, 9-(phenylmethyl)-, bis(1,1-dimethylethyl) ester (9CI) (CA INDEX NAME)



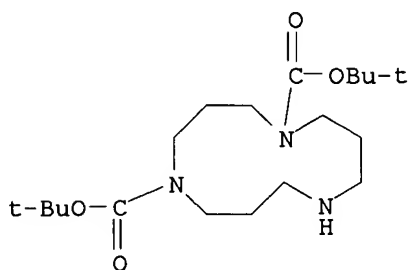
RN 174192-39-3 CAPLUS

CN 1,5,9-Triazacyclododecane-1,5-dicarboxylic acid, 8-cyano-9-hydroxy-, bis(1,1-dimethylethyl) ester (9CI) (CA INDEX NAME)

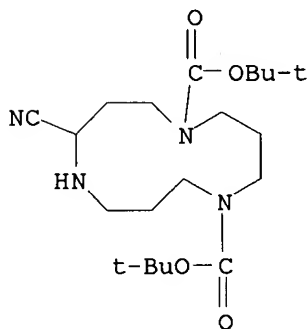


RN 174192-40-6 CAPLUS

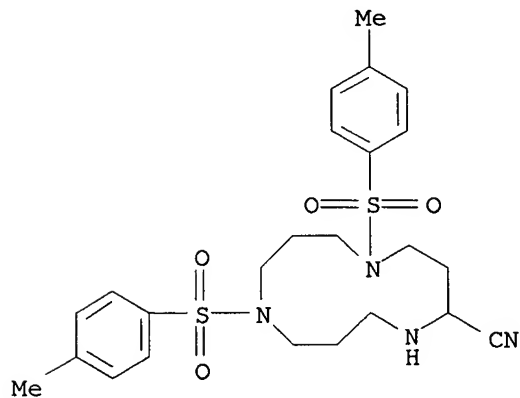
CN 1,5,9-Triazacyclododecane-1,5-dicarboxylic acid, bis(1,1-dimethylethyl) ester (9CI) (CA INDEX NAME)



RN 174192-41-7 CAPLUS
CN 1,5,9-Triazacyclododecane-1,5-dicarboxylic acid, 8-cyano-, bis(1,1-dimethylethyl) ester (9CI) (CA INDEX NAME)



IT 174192-37-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(regioselective oxidative cyanation method for macrocyclic polyamines)
RN 174192-37-1 CAPLUS
CN 1,5,9-Triazacyclododecane-2-carbonitrile, 5,9-bis[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)



180 ANSWER 48 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1996:77520 CAPLUS

DOCUMENT NUMBER: 124:232424

TITLE: Synthesis and characterization of a novel macrocyclic ligand containing nine donor atoms

AUTHOR(S): Giovenzana, G. B.; Jommi, G.; Pagliarin, R.; Sisti, M.; Aime, S.; Botta, M.; Geninatti, Crich, S.

CORPORATE SOURCE: Dip. Chim. Organica Industriale, Milan, I-20133, Italy

SOURCE: Recueil des Travaux Chimiques des Pays-Bas (1996), 115(1), 94-8

CODEN: RTCPA3; ISSN: 0165-0513

PUBLISHER: Elsevier

DOCUMENT TYPE: Journal

LANGUAGE: English

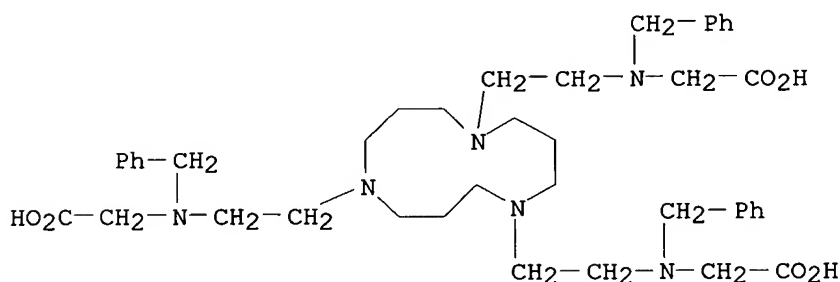
AB The synthesis of a novel macrocyclic ligand containing nine potential coordination sites (six nitrogens and three oxygens) formed by a triazacyclododecane ring trisubstituted with $-\text{CH}_2\text{CH}_2\text{N}(\text{CH}_2\text{Ph})\text{CH}_2\text{COOH}$ groups is reported. The protonation scheme of this ligand has been elucidated by measuring the proton NMR shifts of the various methylenic resonances upon changing the pH of the solution. This ligand affords stable metal complexes with Cd^{2+} ion, whose ^1H - and ^{13}C -NMR spectra suggest a remarkable kinetic inertia and stereochem. rigidity.

IT 174783-36-9P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 174783-36-9 CAPLUS

CN Glycine, N,N',N''-(1,5,9-triazacyclododecane-1,5,9-triyltri-2,1-ethanediyl)tris[N-(phenylmethyl)- (9CI) (CA INDEX NAME)



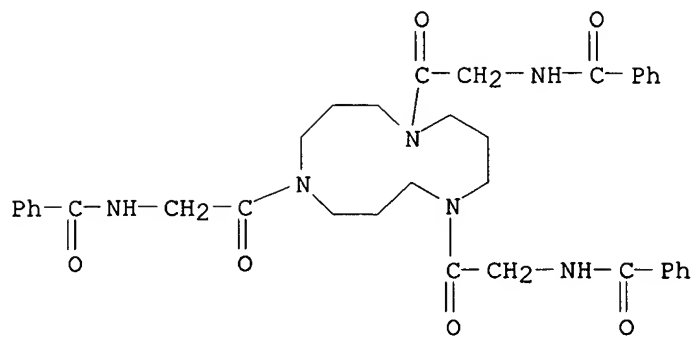
IT 174783-34-7P 174783-35-8P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)

(synthesis and characterization of a novel macrocyclic ligand containing nine donor atoms)

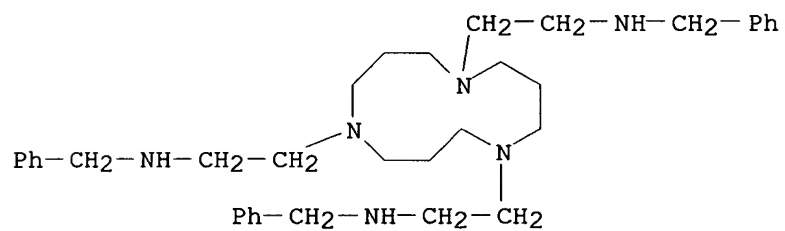
RN 174783-34-7 CAPLUS

CN Benzamide, N,N',N''-[1,5,9-triazacyclododecane-1,5,9-triyltris(2-oxo-2,1-ethanediyl)]tris- (9CI) (CA INDEX NAME)



RN 174783-35-8 CAPLUS

CN 1,5,9-Triazacyclododecane-1,5,9-triethanamine, N,N',N''-tris(phenylmethyl)-
(9CI) (CA INDEX NAME)



130 ANSWER 49 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1995:953685 CAPLUS

DOCUMENT NUMBER: 124:74712

TITLE: Synthesis and coordination chemistry of the pyridyl pendant-arm azamacrocycles 1-(2-pyridylmethyl)-1,5,9-triazacyclododecane L1 and 1-(2-pyridyl-2'-ethyl)-1,5,9-triazacyclododecane L2, with nickel(II), copper(II) and zinc(II). Crystal structures of [Ni(L1)(O₂NO)]NO₃ and [ZnL2][Zn(NO₃)₃·6H₂O·3.67ClO₄·0.33H₂O]

AUTHOR(S): Turonek, Mary L.; Moore, Peter; Clase, Howard J.; Alcock, Nathaniel W.

CORPORATE SOURCE: Dep. Chem., University of Warwick, Coventry, CV4 7AL, UK

SOURCE: Journal of the Chemical Society, Dalton Transactions: Inorganic Chemistry (1995), (22), 3659-66
CODEN: JCDTBI; ISSN: 0300-9246

PUBLISHER: Royal Society of Chemistry

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The azamacrocyclic ligands 1-(2-pyridylmethyl)-1,5,9-triazacyclododecane L1 and 1-(2-pyridyl-2'-ethyl)-1,5,9-triazacyclododecane L2 were prepared, and their complexes with hydrated Ni(II), Cu(II) and Zn(II) nitrates were isolated. The Ni(II) complexes are high spin and six-coordinate, while ¹³C NMR spectroscopy shows that [ZnL1(OH)₂]²⁺ exists as a sym. trigonal bipyramidal isomer in solution, and [ZnL2]²⁺ exists as a 2:1 mixture of tetrahedral and asym. trigonal-bipyramidal isomers. X-ray crystallog. was used to determine the solid-state structures of the octahedral [NiL1(O₂NO)]⁺, and the tetrahedral isomer of [ZnL2]²⁺.

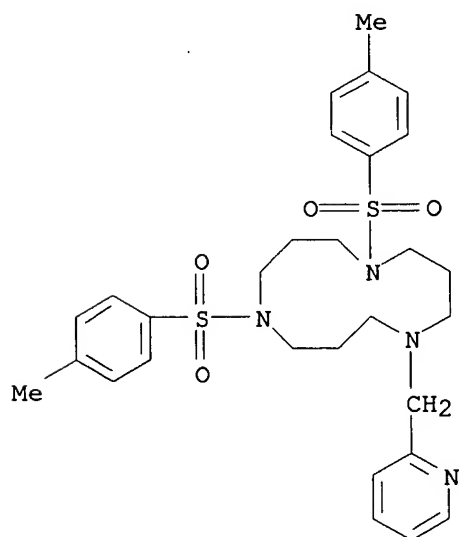
IT 172101-45-0P, 1-(2-Pyridylmethyl)-5,9-bis(toluene-p-sulfonyl)-1,5,9-triazacyclododecane 172101-50-7P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(for preparation of pyridylalkyltriazacyclododecane)

RN 172101-45-0 CAPLUS

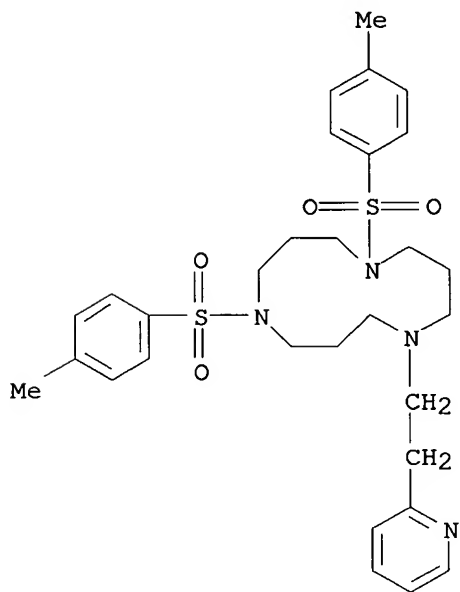
CN 1,5,9-Triazacyclododecane, 1,5-bis[(4-methylphenyl)sulfonyl]-9-(2-pyridinylmethyl)- (9CI) (CA INDEX NAME)



10/680,076

RN 172101-50-7 CAPLUS

CN 1,5,9-Triazacyclododecane, 1,5-bis[(4-methylphenyl)sulfonyl]-9-[2-(2-pyridinyl)ethyl]- (9CI) (CA INDEX NAME)



10/680,076

~~130~~ ANSWER 50 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1995:763501 CAPLUS
DOCUMENT NUMBER: 123:169670
TITLE: Preparation of macrocyclic polyamine derivatives
INVENTOR(S): Iwata, Masaaki
PATENT ASSIGNEE(S): Rikagaku Kenkyuzyo, Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 58 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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JP 06256512	A2	19940913	JP 1993-71147	19930305
PRIORITY APPLN. INFO.:			JP 1993-71147	19930305
OTHER SOURCE(S):	MARPAT	123:169670		
GI				

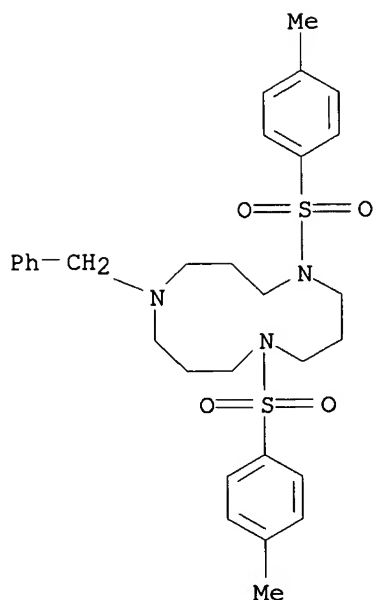
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Macrocyclic polyamines e.g. compds. I (Ts = tosyl) and II (R = Ts, H) and their salts, having biomimetic functions and useful as catalysts (no data), were prepared Thus, stirring N5,N9,N17,N21-tetratosyl-1,5,9,13,17,21-hexaazacyclotetracosane with N1-(3-bromopropyl)-N5,N9-ditosyl-1,5,9-triazacyclododecane and NaHCO3 in MeCN at room temperature for 2 days gave 82% I.

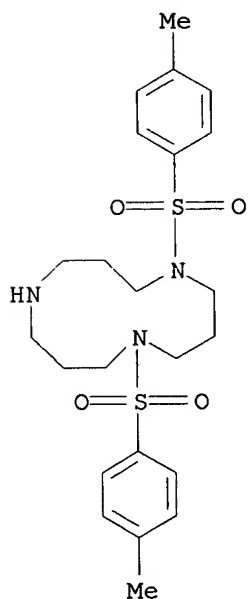
IT 164913-15-9
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of macrocyclic polyamine derivs.)

RN 164913-15-9 CAPLUS

CN 1,5,9-Triazacyclododecane, 1,5-bis[(4-methylphenyl)sulfonyl]-9-(phenylmethyl)- (9CI) (CA INDEX NAME)

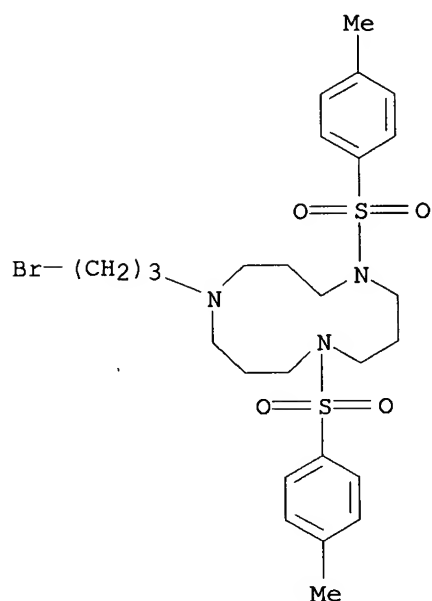


IT 164913-31-9P 164913-40-0P 167080-90-2P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (preparation of macrocyclic polyamine derivs.)
 RN 164913-31-9 CAPLUS
 CN 1,5,9-Triazacyclododecane, 1,5-bis[(4-methylphenyl)sulfonyl]- (9CI) (CA
 INDEX NAME)



RN 164913-40-0 CAPLUS
 CN 1,5,9-Triazacyclododecane, 1-(3-bromopropyl)-5,9-bis[(4-

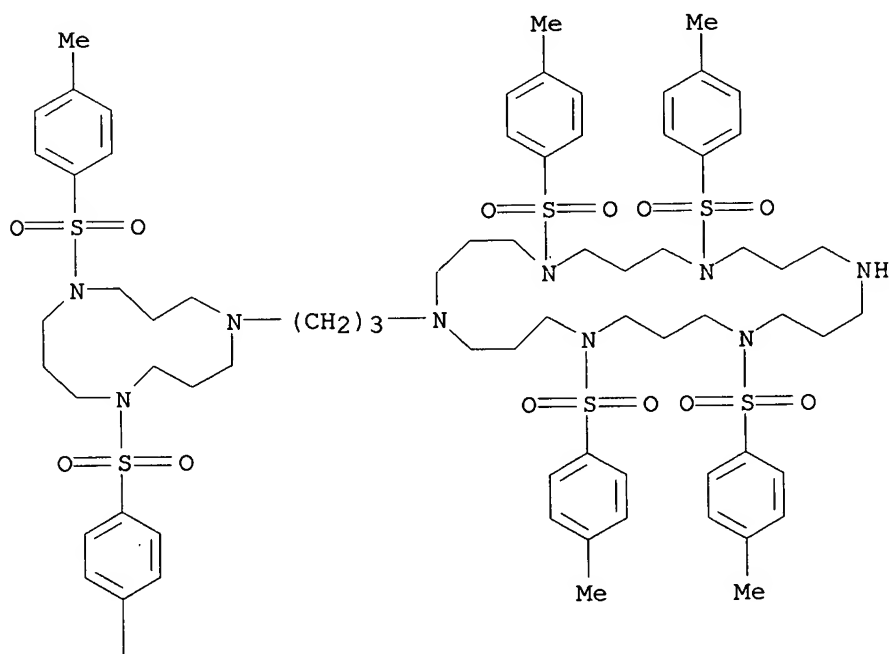
methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)



RN 167080-90-2 CAPLUS

CN 1,5,9,13,17,21-Hexaazacyclotetracosane, 9-[3-[5,9-bis[(4-methylphenyl)sulfonyl]-1,5,9-triazacyclododec-1-yl]propyl]-1,5,13,17-tetrakis[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)

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PAGE 2-A



IT 167080-92-4P 167080-93-5P 167080-94-6P

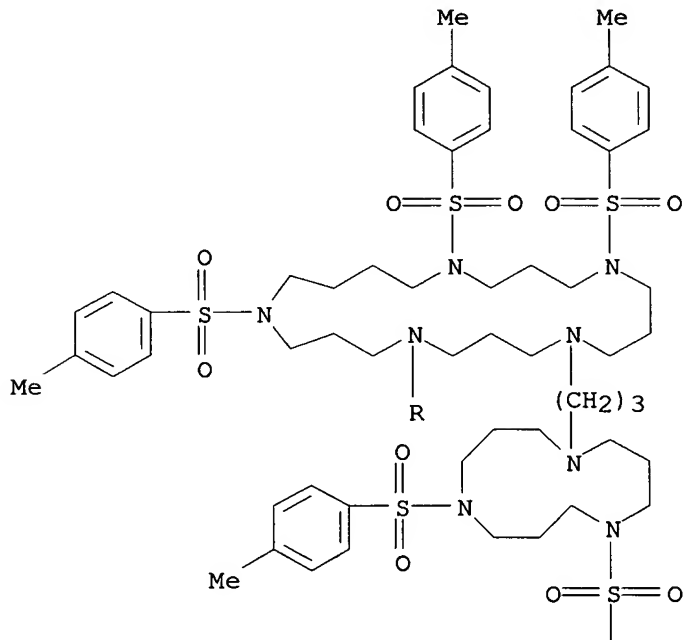
167080-97-9P 167080-99-1P

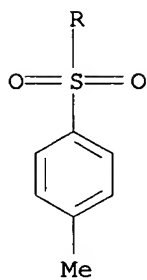
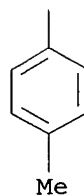
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of macrocyclic polyamine derivs.)

RN 167080-92-4 CAPLUS

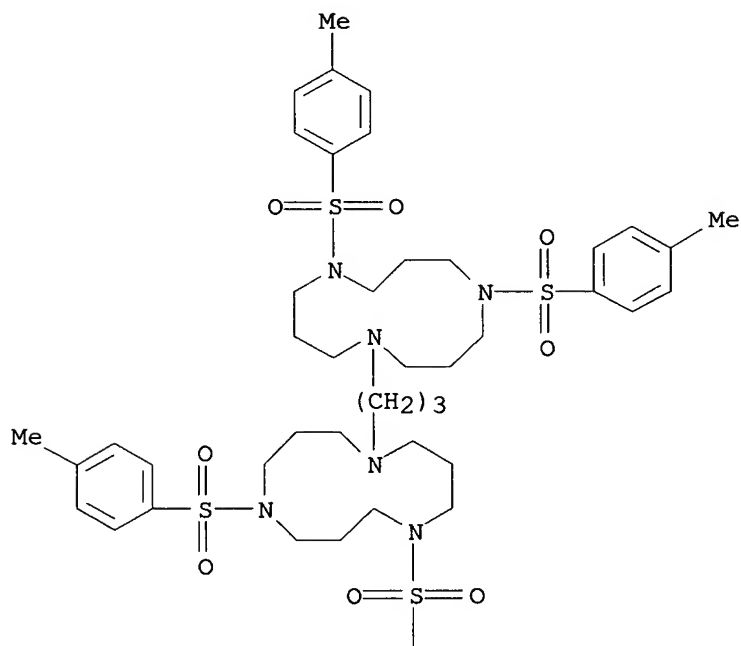
CN 1,5,9,13,17-Pentaazacycloheneicosane, 9-[3-[5,9-bis[(4-methylphenyl)sulfonyl]-1,5,9-triazacyclododec-1-yl]propyl]-1,5,13,17-tetrakis[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)

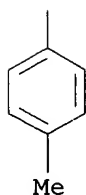
PAGE 1-A





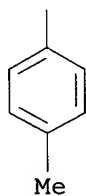
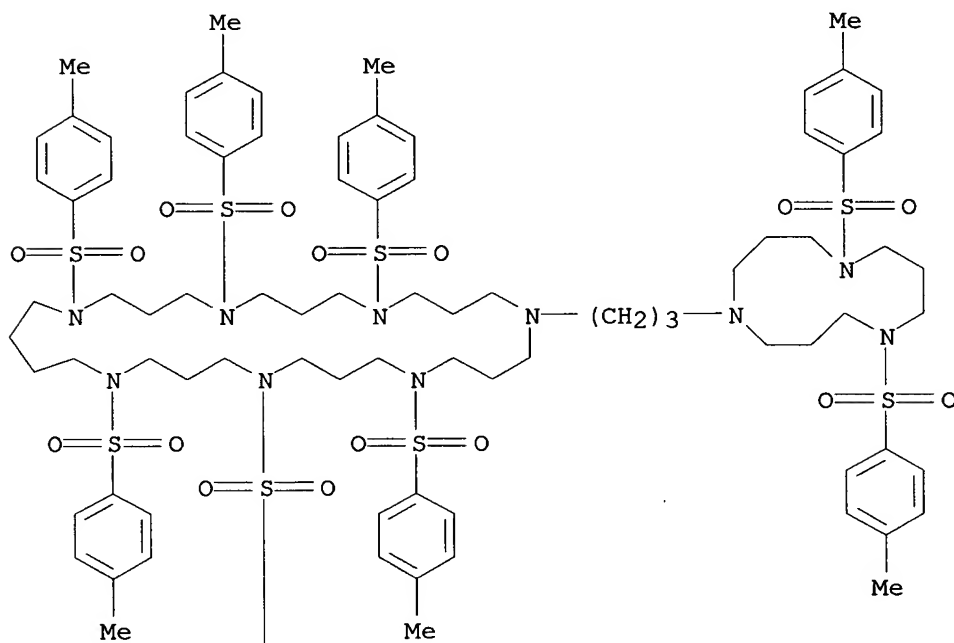
RN 167080-93-5 CAPLUS
 CN 1,5,9-Triazacyclododecane, 1,1'-(1,3-propanediyl)bis[5,9-bis[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)





RN 167080-94-6 CAPLUS

CN 1,5,9,13,17,21,25-Heptaazacyclononacosane, 13-[3-[5,9-bis[(4-methylphenyl)sulfonyl]-1,5,9-triazacyclododec-1-yl]propyl]-1,5,9,17,21,25-hexakis[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)

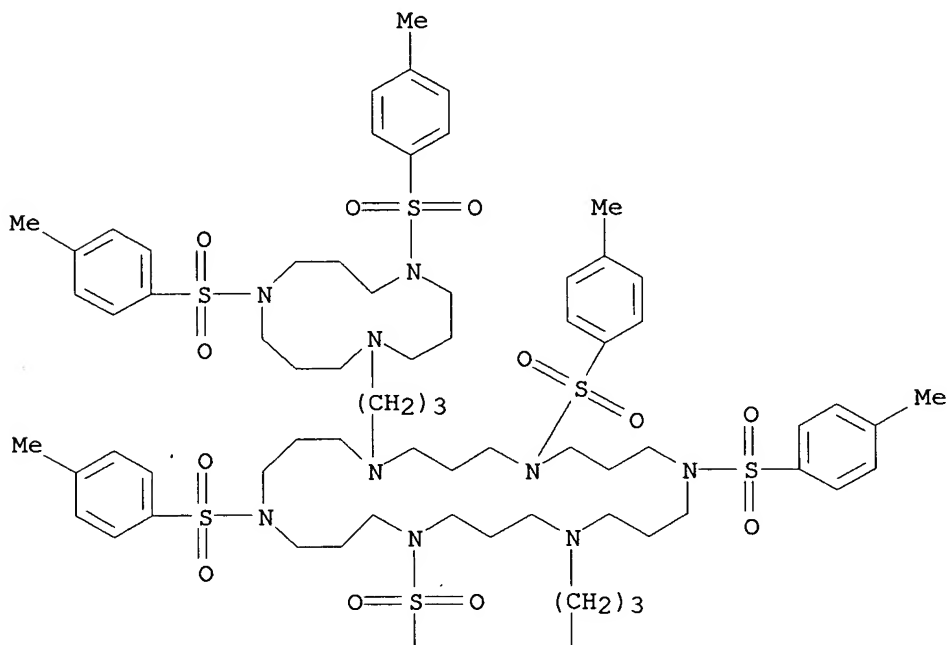


RN 167080-97-9 CAPLUS

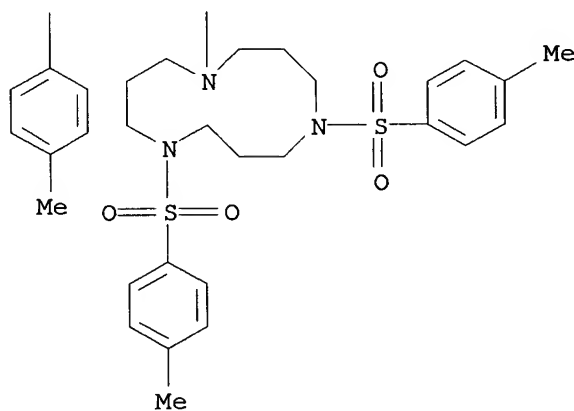
CN 1,5,9,13,17,21-Hexaazacyclotetracosane, 1,13-bis[3-[1,5-bis[(4-

methylphenyl)sulfonyl]-1,5,9-triazacyclododec-9-yl]propyl]-5,9,17,21-tetrakis[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)

PAGE 1-A

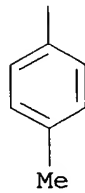
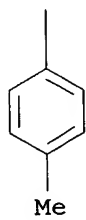
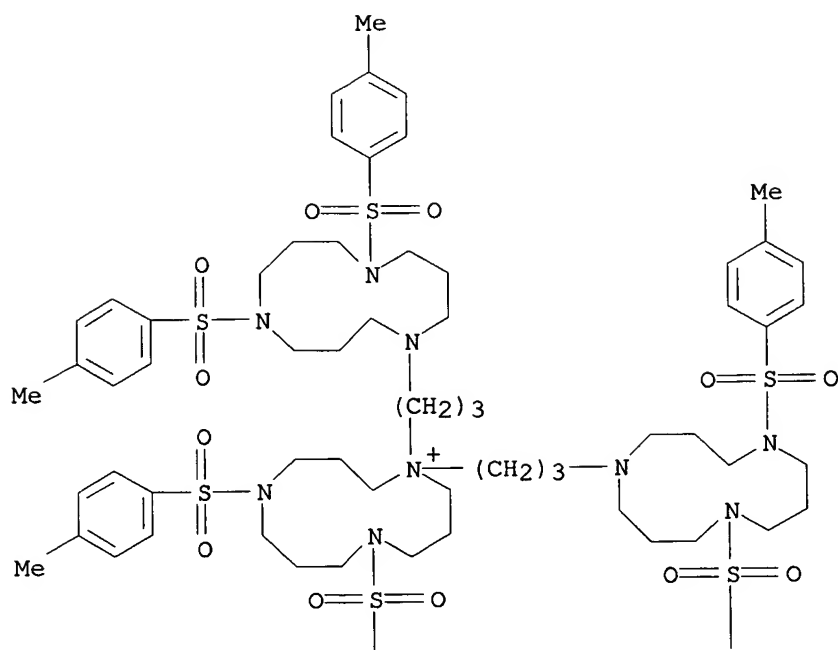


PAGE 2-A



RN 167080-99-1 CAPLUS

CN 5,9-Diaza-1-azoniacyclododecane, 1,1-bis[3-[5,9-bis[(4-methylphenyl)sulfonyl]-1,5,9-triazacyclododec-1-yl]propyl]-5,9-bis[(4-methylphenyl)sulfonyl]-, bromide (9CI) (CA INDEX NAME)



~~L80~~ ANSWER 51 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1995:740701 CAPLUS

DOCUMENT NUMBER: 123:267802

TITLE: Siderophore analogs. Synthesis and chelating properties of a new macrocyclic trishydroxamate ligand

AUTHOR(S): Esteves, M. Alexandra; Vaz, M. Candida T.; Goncalves, M. L. S. Simoes; Farkas, Etelka; Santos, M. Amelia

CORPORATE SOURCE: Cent. Quim. Estrutural, Inst. Superior Tecnico, Lisbon, 1096, Port.

SOURCE: Journal of the Chemical Society, Dalton Transactions: Inorganic Chemistry (1995), (15), 2565-73
CODEN: JCDBTBI; ISSN: 0300-9246

PUBLISHER: Royal Society of Chemistry

DOCUMENT TYPE: Journal

LANGUAGE: English

AB A new Fe(III)-specific ligand, 1,5,9-triazacyclododecane-N,N',N''-tris(N-methylacetohydroxamic acid) H3L, containing three hydroxamic acid groups as pendant arms on a macrocyclic triamine backbone, was synthesized and characterized. Its acid-base and chelating properties with Fe(III) and Cu(II) ions were studied by potentiometric and spectrophotometric techniques. The mechanism of electron transfer as well as the kinetics of dissociation and stability consts. of reduced species, which probably are important in the biol. activity of this siderophore analog, were studied by voltammetric methods. This ligand proved to be biol. active and its properties were compared with ferrichrome and ferrioxamine B.

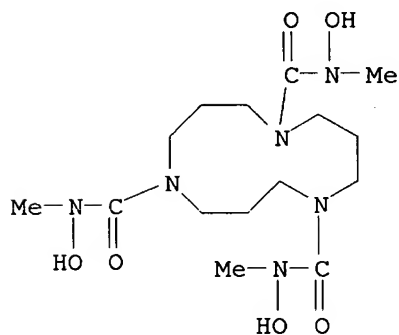
IT 169386-06-5

RL: PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); PROC (Process); RACT (Reactant or reagent)

(synthesis and complexation of new macrocyclic trishydroxamate ligand with iron(3+) and copper(2+))

RN 169386-06-5 CAPLUS

CN 1,5,9-Triazacyclododecane-1,5,9-tricarboxamide, N,N',N''-trihydroxy-N,N',N''-trimethyl- (9CI) (CA INDEX NAME)



L80 ANSWER 52 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1995:677172 CAPLUS

DOCUMENT NUMBER: 123:55936

TITLE: Preparation of intermediates of macrocyclic polyamines

INVENTOR(S): Iwata, Masaaki

PATENT ASSIGNEE(S): Rikagaku Kenkyuzyo, Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 29 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 06211776	A2	19940802	JP 1993-23663	19930119
PRIORITY APPLN. INFO.:			JP 1993-23663	19930119

OTHER SOURCE(S): MARPAT 123:55936

AB Title intermediates e.g. N8-benzyl-N1,N4,N12,N15-tetratosyl-4,8,12-triaza-1,15-pentadecanediamine, O1,O12-dimesyl-N4,N9-ditosyl-4,9-diaza-1,12-dodecanediol, N,N-bis(3-bromopropyl)benzylamine (I), and N5,N10,N14,N18,N22,N27-hexatosyl-1,5,10,14,18,22,27-heptaazacyclotriacontane were prepared Thus, stirring benzylamine with 1,3-dibromopropane and NaHCO₃ in MeCN at 60° for 22 h gave 37% I.

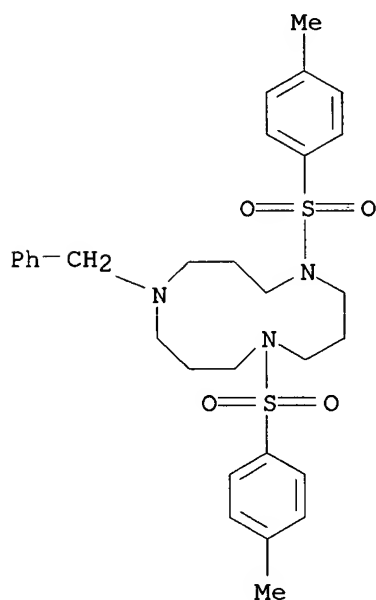
IT 164913-15-9

RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of intermediates of macrocyclic polyamines)

RN 164913-15-9 CAPLUS

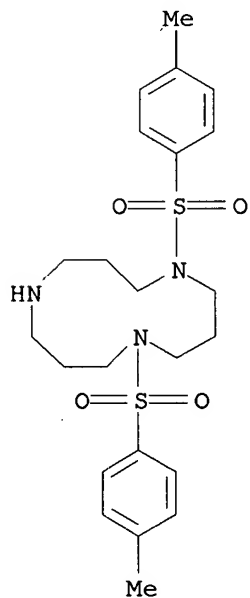
CN 1,5,9-Triazacyclododecane, 1,5-bis[(4-methylphenyl)sulfonyl]-9-(phenylmethyl)- (9CI) (CA INDEX NAME)



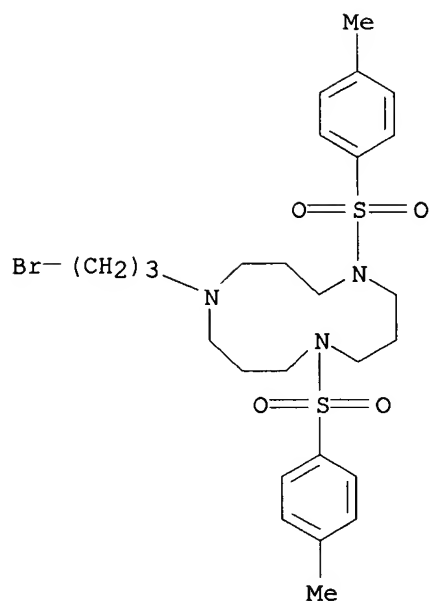
IT 164913-31-9P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of intermediates of macrocyclic polyamines)
 RN 164913-31-9 CAPLUS
 CN 1,5,9-Triazacyclododecane, 1,5-bis[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)



IT 164913-40-0P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of intermediates of macrocyclic polyamines)
 RN 164913-40-0 CAPLUS
 CN 1,5,9-Triazacyclododecane, 1-(3-bromopropyl)-5,9-bis[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)



~~X~~ L30 ANSWER 53 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1995:283587 CAPLUS

DOCUMENT NUMBER: 122:229436

TITLE: Design and Synthesis of Calcium and Magnesium Ionophores Based on Double-Armed Diazacrown Ether Compounds and Their Application to an Ion Sensing Component for an Ion-Selective Electrode

AUTHOR(S): Suzuki, Koji; Watanabe, Kazuhiko; Matsumoto, Yukihiro; Kobayashi, Mitsuru; Sato, Sayaka; Siswanta, Dwi; Hisamoto, Hideaki

CORPORATE SOURCE: Department of Applied Chemistry, Keio University, Yokohama, 223, Japan

SOURCE: Analytical Chemistry (1995), 67(2), 324-34
CODEN: ANCHAM; ISSN: 0003-2700

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The double-armed diazacrown ethers, which have a base diazacrown ether ring with two diamide-type side chains, were designed and synthesized from the proposed mol. model for the novel neutral Ca²⁺ and Mg²⁺ ionophores. The potentiometric ion-selective electrodes were prepared with over 20 kinds of systematically synthesized diazacrown ether derivs. The relation between the mol. structures of the ionophores and the ion selectivities was fully discussed. The electrodes based on the 21- and 18-membered diazacrown ether derivs. possessing a glycolic diamide and malonic diamide in their side chains (K23E1 and K22B5) exhibited excellent Ca²⁺ and Mg²⁺ selectivities, resp. The ion-selectivity features of the novel Ca²⁺ and Mg²⁺ ionophores supply important structural information about the design of host mols. for alkaline earth metal cations.

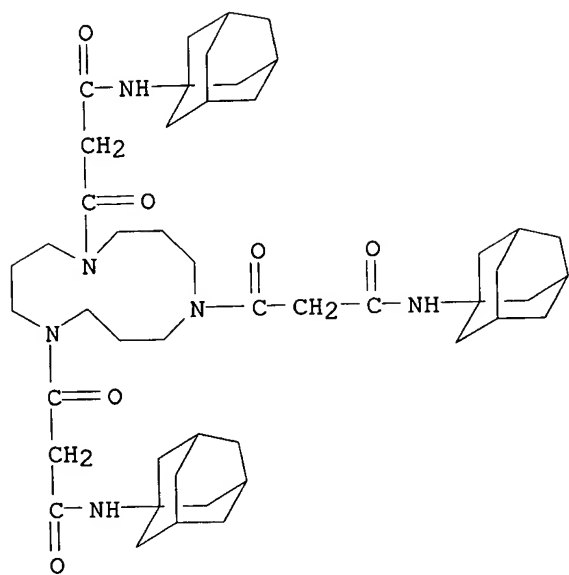
IT 162008-35-7P, 1,5,9-Tris[(N-(1-adamantyl)carbamoyl)acetyl]-1,5,9-triazacyclododecane

RL: ARU (Analytical role, unclassified); DEV (Device component use); PNU (Preparation, unclassified); PRP (Properties); ANST (Analytical study); PREP (Preparation); USES (Uses)

(design and synthesis of calcium and magnesium ionophores based on double-armed diazacrown ether compds. and application to ion sensing component for ion-selective electrode)

RN 162008-35-7 CAPLUS

CN 1,5,9-Triazacyclododecane-1,5,9-tripropanamide, β,β',β'' -trioxo-N,N',N''-tris(tricyclo[3.3.1.1^{3,7}]dec-1-yl)- (9CI) (CA INDEX NAME)



130 ANSWER 54 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1995:64905 CAPLUS

DOCUMENT NUMBER: 122:44835

TITLE: Synthesis, Characterization, and Molecular Mechanics

Studies on the Metal Complexes of 1,5,9-Tris(2-pyridylmethyl)-1,5,9-triazacyclododecane, [ML1](PF6)2 (M = Fe(II), Mn(II), Co(II), Ni(II), Cu(II), Pd(II))

AUTHOR(S): Zhang, Delong; Busch, Daryle H.

CORPORATE SOURCE: Department of Chemistry, University of Kansas, Lawrence, KS, 66045, USA

SOURCE: Inorganic Chemistry (1994), 33(22), 5138-43
CODEN: INOCAJ; ISSN: 0020-1669

DOCUMENT TYPE: Journal

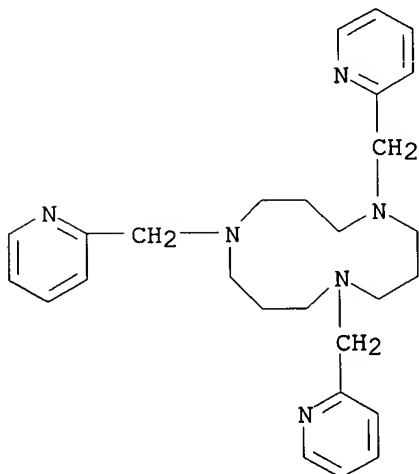
LANGUAGE: English

AB 1,5,9-Tris(2-pyridylmethyl)-1,5,9-triazacyclododecane (L1) and [ML1](PF6)2 (M = Fe(II), Mn(II), Co(II), Ni(II), Cu(II), Pd(II)), were prepared and characterized. The effective magnetic moments at room temperature are 5.68, 6.004.38, 3.23, and 2.10 μ_B , resp., for the Fe(II), Mn(II), Co(II), Ni(II), and Cu(II) complexes, and Pd(II) complex is diamagnetic. Cyclic voltammetry provided the potentials for the quasireversible redox couples Fe(III)/Fe(II) and Mn(III)/Mn(II) and for the reversible couples Cu(II)/Cu(I) and Pd(II)/Pd(I): 1.22, 1.48, -0.21, and -0.77 V, resp. [CoIIIL1]2+, [NiIIIL1]2+, and [PdIIIL1]2+ are irreversibly oxidized at 1.49, 1.9, and 1.27 V vs. normal H electrode. The new complexes are much more resistant to oxidation than the analogous derivs. of 1,4,7-tris(2-pyridylmethyl)-1,4,7-triazacyclononane. This difference in behavior is rationalized from mol. mechanics calcns. that show the min. strain energy M-N(sp3) distances to be 2.37 Å for a 1,5,9-tris(2-pyridylmethyl)-1,5,9-triazacyclododecane complex and 2.12 Å for a 1,4,7-tris(2-pyridylmethyl)-1,4,7-triazacyclononane complex. The influence of the triaza ring size on the phys. properties of the complexes is also discussed.

IT 102851-51-4, 1,5,9-Tris(2-pyridylmethyl)-1,5,9-triazacyclododecane
RL: RCT (Reactant); RACT (Reactant or reagent)
(for preparation of transition metal homoleptic complexes)

RN 102851-51-4 CAPLUS

CN 1,5,9-Triazacyclododecane, 1,5,9-tris(2-pyridinylmethyl)- (9CI) (CA INDEX NAME)



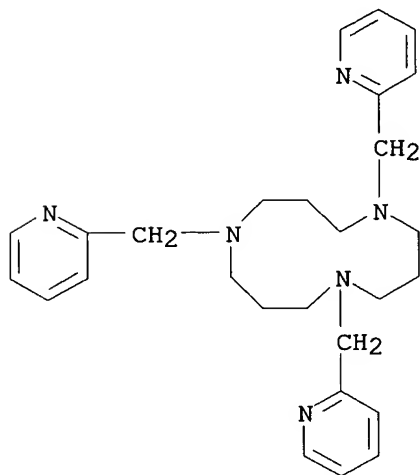
10/680,076

IT 102851-51-4DP, palladium complex

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and cyclic voltammetry and mol. mech. calcns. for coordinate
bond strain energy of)

RN 102851-51-4 CAPLUS

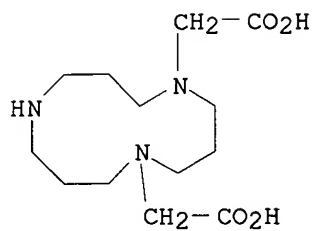
CN 1,5,9-Triazacyclododecane, 1,5,9-tris(2-pyridinylmethyl)- (9CI) (CA INDEX
NAME)



L80 ANSWER 55 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN
 ACCESSION NUMBER: 1994:534168 CAPLUS
 DOCUMENT NUMBER: 121:134168
 TITLE: Preparation of N-substituted-polyazamacrocycles as
 chelants
 INVENTOR(S): Sherry, A. Dean; Van Westrenen, Jeroen
 PATENT ASSIGNEE(S): Board of Regents, the University of Texas System, USA
 SOURCE: U.S., 40 pp. Cont.-in-part of U.S. Ser. No. 615,619.
 CODEN: USXXAM
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 8
 PATENT INFORMATION:

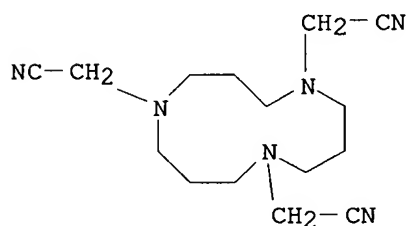
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5316757	A	19940531	US 1991-808845	19911213
US 4639365	A	19870127	US 1984-662075	19841018
US 4983376	A	19910108	US 1988-291053	19881228
US 5342606	A	19940830	US 1990-615619	19901119
WO 9312097	A1	19930624	WO 1992-US9247	19921027
W: AT, AU, BB, BG, BR, CA, CH, CS, DE, DK, ES, FI, GB, HU, JP, KP, KR, LK, LU, MG, MN, MW, NL, NO, PL, RO, RU, SD, SE				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, SN, TD, TG				
AU 9229124	A1	19930719	AU 1992-29124	19921027
AU 659244	B2	19950511		
EP 618910	A1	19941012	EP 1992-923096	19921027
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, SE				
ZA 9208338	A	19930504	ZA 1992-8338	19921028
CN 1073680	A	19930630	CN 1992-114146	19921211
CN 1033803	B	19970115		
US 5428155	A	19950627	US 1994-250048	19940527
PRIORITY APPLN. INFO.:			US 1984-662075	A2 19841018
			US 1987-7729	A2 19870127
			US 1988-291053	A2 19881228
			US 1989-357193	B2 19890525
			US 1990-615619	A2 19901119
			US 1991-808845	A 19911213
			WO 1992-US9247	A 19921027

OTHER SOURCE(S): MARPAT 121:134168
 AB Title compds. [e.g., 1,4,7,10-tetraazacyclododecane(N,N''-diacetic acid)(N'R1)(N''R2); R1,R2 = H, CH2CH2OH, CH2CHMeOH, CH2P(O)Et(O-), CH2P(O)(OEt)(O-), CH2PO32-] were prepared as chelants for MRI contrast agents and NMR shift reagents (no data). Thus, 1,4,7,10-tetraazacyclododecane was heated at 40° for 16h in aqueous solution with HCHO.Na2SO3 and the product treated with NaCN to give, after HCl hydrolysis, 1,4,7,10-tetraazacyclododecane-N,N''-diacetic acid hydrochloride.
 IT 127603-37-6P 144003-25-8P 157282-08-1P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of, in preparation of chelant)
 RN 127603-37-6 CAPLUS
 CN 1,5,9-Triazacyclododecane-1,5-diacetic acid (9CI) (CA INDEX NAME)



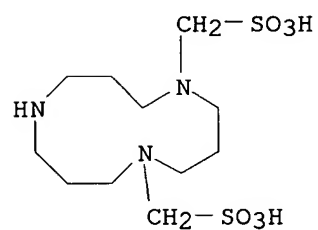
RN 144003-25-8 CAPLUS

CN 1,5,9-Triazacyclododecane-1,5,9-triacetonitrile (9CI) (CA INDEX NAME)



RN 157282-08-1 CAPLUS

CN 1,5,9-Triazacyclododecane-1,5-dimethanesulfonic acid, disodium salt, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

●2 Na

L80 ANSWER 56 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1994:245575 CAPLUS

DOCUMENT NUMBER: 120:245575

TITLE: Study of the transamidative ring expansion of N- ω -halogenoalkyl- β -lactams of alkyl chain lengths 2-12 in liquid ammonia and other liquid amines: syntheses of 7-, 8- and 9-membered 1,5-diazacyclic ketones, including routes to (\pm)-dihydroperiphylline and (\pm)-celabenzine

AUTHOR(S): Begley, Michael J.; Crombie, Leslie; Daigh, David; Jones, Raymond C. F.; Osborne, Steven; Webster, Richard A. B.

CORPORATE SOURCE: Dep. Chem., Univ. Nottingham, Nottingham, NG7 2RD, UK

SOURCE: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (1993), (17), 2027-46

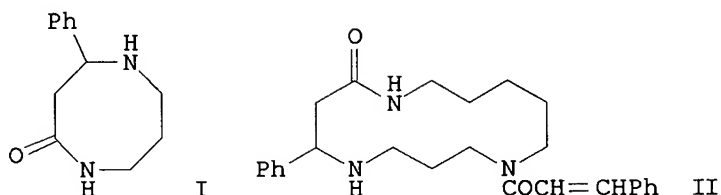
CODEN: JCPRB4; ISSN: 0300-922X

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 120:245575

GI



AB N-(3-halogenopropyl)-4-phenylazetidin-2-ones undergo amination in liquid ammonia followed by transamidative ring expansion to give the eight-membered 4-phenyl-1,5-diazacyclooctan-2-one (I) in excellent yield. Ring expansion of the amines in liquid ammonia is found to be much more effective than in hydrocarbon solvents. Formation of 7-, 8-, and 9-membered azalactams from the requisite ω -halogenoalkyl- β -lactams is an excellent synthetic process, though it is not applicable to 10-membered rings. In the cases of rings of 13-, 15- and 17-members, although amination and apparent expansion takes place, the large rings appear not to be stable to ammonia and the final products are acyclic amids. N-[4-halogenobut-2(Z)-enyl]-4-phenylazetidin-2-one satisfactorily forms a 9-membered (Z)-olefinic azalactam, but the (E)-isomer gives an acyclic amino amide. By using alkyl-substituted β -lactam side-chains, C-substituted medium rings can be obtained; the relative instability of N-acyl β -lactams to ammonia, however, leads to acylamino amides rather than expanded rings. Employing ethylamine in place of ammonia, N-ethylated azalactams are formed satisfactorily, and using allylamine, N-allyl medium rings capable of further elaboration are obtained. The chemical of these systems is discussed. Using transamidation in liquid ammonia, a short synthesis of the 9-membered sperimidine alkaloid (\pm)-dihydroperiphylline (II) was achieved. Synthesis of key intermediates, whose transformation into the 13-membered alkaloids of the celabenzine group has already been effected, has been carried out. X-ray single-crystal structure detns. for 4-phenyl-1,5-diazacyclononan-2-one, trans-4-phenyl-8-methyl-1,5-diazacyclooctan-2-one and (Z)-4-phenyl-1,5-

10/680,076

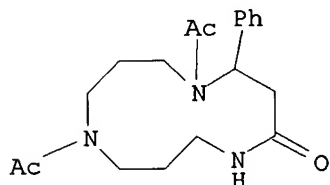
diazacyclonon-7-en-2-one are reported, and comment is made on certain conformational features.

IT 154218-98-1

RL: RCT (Reactant); RACT (Reactant or reagent)
(intermediate, preparation of diazacyclic ketone)

RN 154218-98-1 CAPLUS

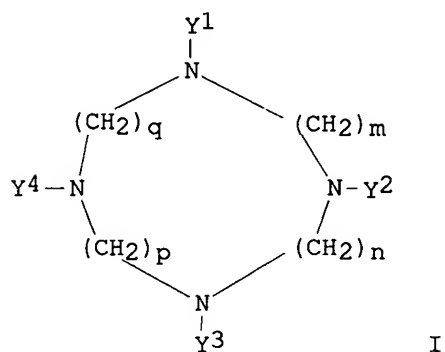
CN 1,5,9-Triazacyclododecan-2-one, 5,9-diacetyl-4-phenyl- (9CI) (CA INDEX NAME)



L30 ANSWER 57 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN

X
 ACCESSION NUMBER: 1994:44581 CAPLUS
 DOCUMENT NUMBER: 120:44581
 TITLE: Synthesis of polyazamacrocycles with more than one type of side-chain chelating groups
 INVENTOR(S): Sherry, A. Dean; Van, Westrenen Jeroen
 PATENT ASSIGNEE(S): University of Texas System, USA
 SOURCE: PCT Int. Appl., 105 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 8
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9312097	A1	19930624	WO 1992-US9247	19921027
W: AT, AU, BB, BG, BR, CA, CH, CS, DE, DK, ES, FI, GB, HU, JP, KP, KR, LK, LU, MG, MN, MW, NL, NO, PL, RO, RU, SD, SE				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, SN, TD, TG				
US 5316757	A	19940531	US 1991-808845	19911213
AU 9229124	A1	19930719	AU 1992-29124	19921027
AU 659244	B2	19950511		
EP 618910	A1	19941012	EP 1992-923096	19921027
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, SE				
PRIORITY APPLN. INFO.:			US 1991-808845	A 19911213
			US 1984-662075	A2 19841018
			US 1987-7729	A2 19870127
			US 1988-291053	A2 19881228
			US 1989-357193	B2 19890525
			US 1990-615619	A2 19901119
			WO 1992-US9247	A 19921027
OTHER SOURCE(S):			MARPAT 120:44581	
GI				



AB The pH controlled selectivity of the sulfomethylation reaction is used to prepare a series of di-, tri-, tetra- and hexaazacyclomacrocycles with specified patterns of pendent side-chain chelating groups. The prepared mono and diacetic acid derivs. together with monomethylenephosphonate and

monomethylenephosphinate derivs. of [12]ane N4, [12]aneN3 and [9]aneN3, make these types of ligands easily available by a synthetic pathway that avoids the use of protective groups. A variety of compds., methods and uses are described. Relatively high synthetic yields are reported of polyazamacrocyclic ligands exhibiting a wide and predictable choice of metal ion binding consts. and water and lipid solubilities by reason of their substituent pendent groups. Application is indicated for MRI contrast agents and NMR shift reagents. A method is described for producing a tetraazamacrocyclic with selectively N-substituted pendent methylenesulfonate groups having a formula I, where m, n, p and q are independently 2 or 3, and where Y1, Y2, Y3 and Y4 are H or CRyRzSO3-, and at least one of Y1, Y2, Y3 and Y4 is CRyRzSO3-, the method comprising obtaining pKa's for nitrogens of a precursor tetraazamacrocyclic where Y1, Y2, Y3 and Y4 are H; reacting, in an aqueous solution having a pH between the lowest pKa of nitrogens to be protonated but not substituted, and the highest pKa of nitrogens to be non-protonated and selectively substituted, the precursor tetraazamacrocyclic with a substitution reagent having a formula X-CRyRzSO3- to produce a tetraazamacrocyclic with selectively substituted pendent methylenesulfonate groups; wherein X is a leaving group subject to displacement by a non-protonated nitrogen of the precursor tetraazamacrocyclic and wherein Ry and Rz are independently hydrogen, alkyl, aryl, alkyl acid, alkyl ether, alkyl ester, or alkyl alc.

IT 144003-16-7P 144003-25-8P 150263-68-6P

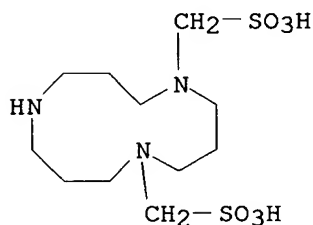
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and reaction of, in polyazamacrocyclic preparation for complexes for

magnetic resonance imaging contrast agents and NMR shift reagent)

RN 144003-16-7 CAPLUS

CN 1,5,9-Triazacyclododecane-1,5-dimethanesulfonic acid, disodium salt (9CI)
(CA INDEX NAME)

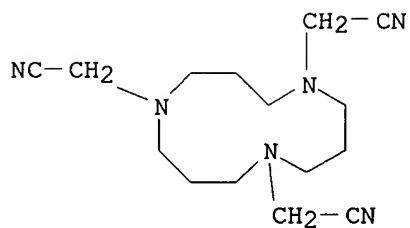


⊙2 Na

RN 144003-25-8 CAPLUS

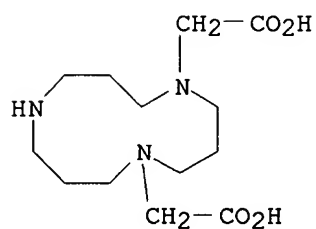
CN 1,5,9-Triazacyclododecane-1,5,9-triacetonitrile (9CI) (CA INDEX NAME)

10/680,076



RN 150263-68-6 CAPLUS

CN 1,5,9-Triazacyclododecane-1,5-diacetic acid, hydrochloride (2:5) (9CI)
(CA INDEX NAME)



●5/2 HCl

10/680,076

L30 ANSWER 58 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1993:182041 CAPLUS

DOCUMENT NUMBER: 118:182041

TITLE: Triazacyclane-based trithiols and their use in the preparation of site-differentiated iron-sulfur clusters

AUTHOR(S): Evans, David J.; Garcia, Gabriel; Leigh, G. Jeffery; Newton, Maurice S.; Santana, M. Dolores

CORPORATE SOURCE: Inst. Plant Sci. Res., Univ. Sussex, Brighton, BN1 9RQ, UK

SOURCE: Journal of the Chemical Society, Dalton Transactions: Inorganic Chemistry (1972-1999) (1992), (22), 3229-34
CODEN: JCDTBI; ISSN: 0300-9246

DOCUMENT TYPE: Journal

LANGUAGE: English

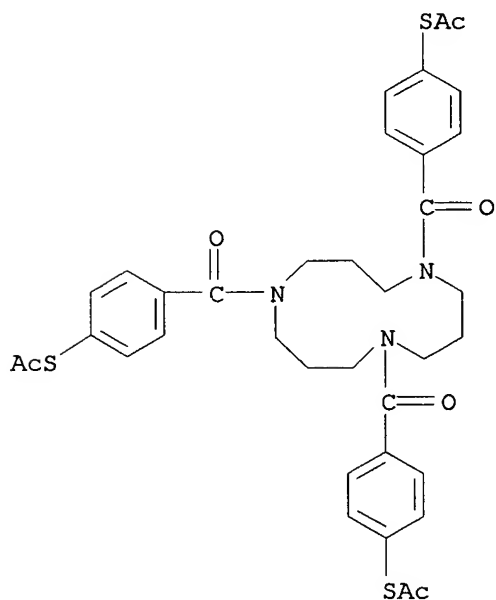
AB The new tripodal thiol ligands 1,4,7-tris(4-mercaptobenzoyl)-1,4,7-triazacyclononane (H3L) and 1,5,9-tris(4-mercaptobenzoyl)-1,5,9-triazacyclododecane were prepared and characterized. On reaction with Fe-S clusters $[\text{Fe}_4\text{S}_4(\text{SR})_4]^{2-}$ ($\text{R} = \text{Et}$ or CMe_3), subsite-differentiated clusters, e.g. $[\text{Fe}_4\text{S}_4\text{L}(\text{SEt})]^{2-}$, were formed. Site-specific reaction at the differentiated Fe is demonstrated. The novel clusters were prepared both in solution and as isolated solids, and characterized mainly by ^1H NMR and Moessbauer spectroscopy.

IT 146070-03-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and hydrolysis of)

RN 146070-03-3 CAPLUS

CN Ethanethioic acid, S,S',S''-[1,5,9-triazacyclododecane-1,5,9-triyltris(carbonyl-4,1-phenylene)] ester (9CI) (CA INDEX NAME)



IT 146070-05-5P, 1,5,9-Tris(4-mercaptobenzoyl)-1,5,9-triazacyclododecane

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

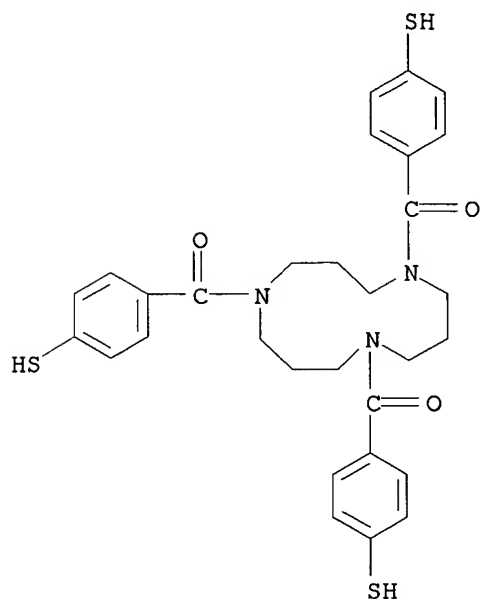
10/680,076

(Reactant or reagent)

(preparation and substitution reaction of, with iron-sulfur thiolato clusters)

RN 146070-05-5 CAPLUS

CN 1,5,9-Triazacyclododecane, 1,5,9-tris(4-mercaptobenzoyl)- (9CI) (CA INDEX NAME)



130 ANSWER 59 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1992:612468 CAPLUS

DOCUMENT NUMBER: 117:212468

TITLE: Sulfomethylation of di-, tri-, and polyazamacrocycles:
a new route to entry of mixed-side-chain macrocyclic
chelates

AUTHOR(S): Van Westrenen, Jeroen; Sherry, A. Dean

CORPORATE SOURCE: Dep. Chem., Univ. Texas, Dallas, Richardson, TX,
75083-0688, USA

SOURCE: Bioconjugate Chemistry (1992), 3(6), 524-32

CODEN: BCCHES; ISSN: 1043-1802

DOCUMENT TYPE: Journal

LANGUAGE: English

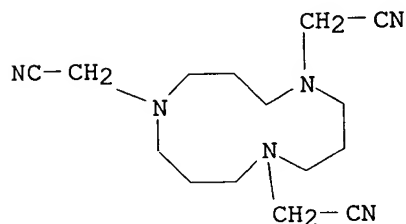
AB The N-sulfomethylation of piperazine and the polyaza macrocycles, [9]aneN3, [12]aneN3, [12]aneN4, and [18]aneN6 with formaldehyde bisulfite in aqueous medium at various pH values is described. The number of methanesulfonate groups introduced into these structures was found to be largely determined by pH. At neutral pH, disubstituted products of [9]aneN3, [12]aneN3, [12]aneN4 are formed and, in the latter case, the trans-1,7-bis(methanesulfonate) isomer was predominant. Similarly, a single, sym. trisubstituted product was formed with [18]aneN6 at neutral pH. Monomethanesulfonated products of these same polyaza compds. were formed at more acidic pH's. These sulfomethylated products were used as an entry into a series of mono- and diacetate, phosphonate, and phosphinate derivs. of [9]aneN3, [12]aneN3, and [12]aneN4. The sulfonate groups may be converted to acetates without isolation of intermediates by using cyanide to displace the sulfonate(s) followed by acidic hydrolysis. The aminomethanesulfonates may also be oxidatively hydrolyzed by using aqueous triiodide as a prelude to the preparation of aminomethanephosphonates or aminomethanephosphinates.

IT 144003-25-8P 144003-27-0P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

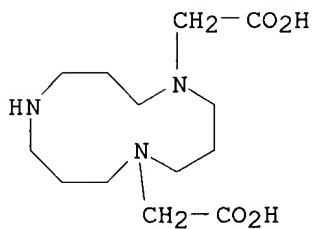
RN 144003-25-8 CAPLUS

CN 1,5,9-Triazacyclododecane-1,5,9-triacetonitrile (9CI) (CA INDEX NAME)



RN 144003-27-0 CAPLUS

CN 1,5,9-Triazacyclododecane-1,5-diacetic acid, monohydrochloride (9CI) (CA
INDEX NAME)



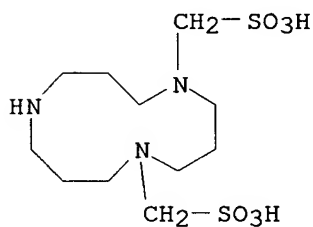
● HCl

IT 144003-16-7P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation, substitution with cyanide, and hydrolysis of, aminoacetate from)

RN 144003-16-7 CAPLUS

CN 1,5,9-Triazacyclododecane-1,5-dimethanesulfonic acid, disodium salt (9CI)
(CA INDEX NAME)



●2 Na

130 ANSWER 60 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1992:227097 CAPLUS

DOCUMENT NUMBER: 116:227097

TITLE: Preparation of terephthaloyl and dansyl derivatives of cyclic polyamines and their complexing abilities for metal ions

AUTHOR(S): Fujiwara, Manabu; Matsushita, Takayuki; Wakita, Hisanobu

CORPORATE SOURCE: Fac. Sci. Technol., Ryukoku Univ., Otsu, 520-21, Japan

SOURCE: Analytical Sciences (1991), 7(Suppl., Proc. Int.

Congr. Anal. Sci., 1991, Pt. 1), 321-4

CODEN: ANSCEN; ISSN: 0910-6340

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Three polymeric ligands containing 9-, 10-, and 12-membered cyclic triamines and four dansyl derivs. of 9-membered cyclic triamine and 12- and 14-membered cyclic tetraamines have been prepared The polymeric ligands can adsorb a copper(II) ion selectively under heterogeneous conditions, and the dansyl derivs. can be applied as a fluorescent reagent to the determination of

silver(I) and copper(II) ions.

IT 141124-32-5P

RL: SPN (Synthetic preparation); PREP (Preparation)

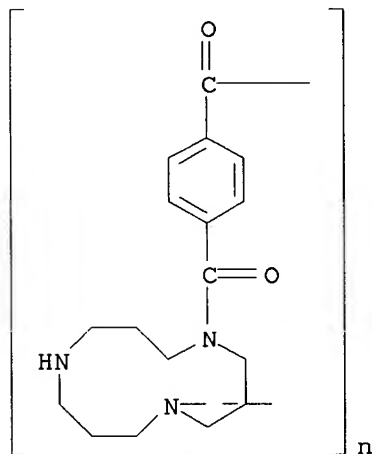
(preparation and fluorescence linewidth of, for adsorption and

determination of

metal ions)

RN 141124-32-5 CAPLUS

CN Poly(1,5,9-triazacyclododecane-1,5-diylcarbonyl-1,4-phenylenecarbonyl)
(9CI) (CA INDEX NAME)



10/680,076

180 ANSWER 61 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1992:214480 CAPLUS

DOCUMENT NUMBER: 116:214480

TITLE: New synthetic routes to macrocyclic triamines

AUTHOR(S): Alder, Roger W.; Mowlam, Rodney W.; Vachon, David J.;
Weisman, Gary R.

CORPORATE SOURCE: Sch. Chem., Univ. Bristol, Bristol, BS8 1TS, UK

SOURCE: Journal of the Chemical Society, Chemical

Communications (1992), (6), 507-8

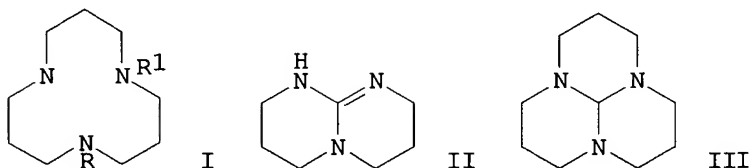
CODEN: JCCCAT; ISSN: 0022-4936

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 116:214480

GI



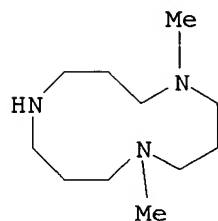
AB 1,5,9-Triazacyclododecane I (R = R1 = H) and related macrocyclic triamines can be conveniently constructed around a single carbon atom as template; this route permits the preparation of selectively alkylated derivs. Thus, the reaction of bicyclic guanidine II with 1,3-dibromopropane, followed by reduction of the tricyclic guanidinium salt with LiAlH₄ gave orthoamide III. Acid-catalyzed hydrolysis of III gave I (R = R1 = H). Methylation of III with MeI, followed by base-catalyzed hydrolysis gave III (R = Me, R1 = H). Methylation of III with MeI, followed by NaBH₄ reduction gave III (R = R1 = Me).

IT 139258-69-8P 141081-92-7P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

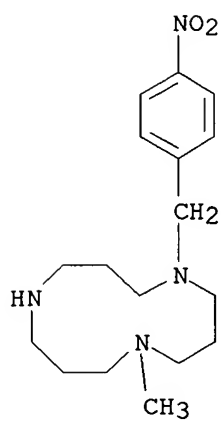
RN 139258-69-8 CAPLUS

CN 1,5,9-Triazacyclododecane, 1,5-dimethyl- (9CI) (CA INDEX NAME)



RN 141081-92-7 CAPLUS

CN 1,5,9-Triazacyclododecane, 1-methyl-5-[(4-nitrophenyl)methyl]- (9CI) (CA INDEX NAME)



10/680,076

180 ANSWER 62 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1992:106266 CAPLUS

DOCUMENT NUMBER: 116:106266

TITLE: Fragmentation during the formic acid/formaldehyde (Eschweiler-Clarke) methylation of polyamines

AUTHOR(S): Alder, Roger W.; Colclough, David; Mowlam, Rodney W.

CORPORATE SOURCE: Sch. Chem., Univ. Bristol, Bristol, BS8 1TS, UK

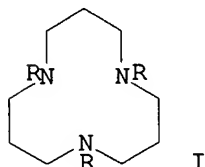
SOURCE: Tetrahedron Letters (1991), 32(52), 7755-8

CODEN: TELEAY; ISSN: 0040-4039

DOCUMENT TYPE: Journal

LANGUAGE: English

GI



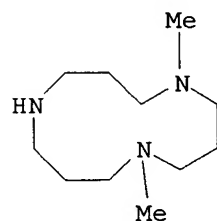
AB Eschweiler-Clarke methylations of both acyclic and cyclic polyamines can lead to methylation products of fragments of the original polyamine. Thus, $\text{H}_2\text{N}(\text{CH}_2)_3\text{NH}(\text{CH}_2)_3\text{NH}(\text{CH}_2)_3\text{NH}_2$ yields $\text{Me}_2\text{N}(\text{CH}_2)_3\text{NMe}_2$ exclusively and 1,5,9-triazacyclododecane (I, R = H) gives 45% I (R = Me) and 45% $\text{Me}_2\text{N}(\text{CH}_2)_3\text{NMe}(\text{CH}_2)_3\text{NMe}_2$.

IT 139258-69-8

RL: RCT (Reactant); RACT (Reactant or reagent)
(Eschweiler-Clarke methylation of)

RN 139258-69-8 CAPLUS

CN 1,5,9-Triazacyclododecane, 1,5-dimethyl- (9CI) (CA INDEX NAME)



10/660,076

130 ANSWER 63 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1992:7618 CAPLUS

DOCUMENT NUMBER: 116:7618

TITLE: Synthetic leather sheets having good feel and their manufacture

INVENTOR(S): Tanaka, Noriyuki

PATENT ASSIGNEE(S): Kuraray Co., Ltd., Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 5 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent

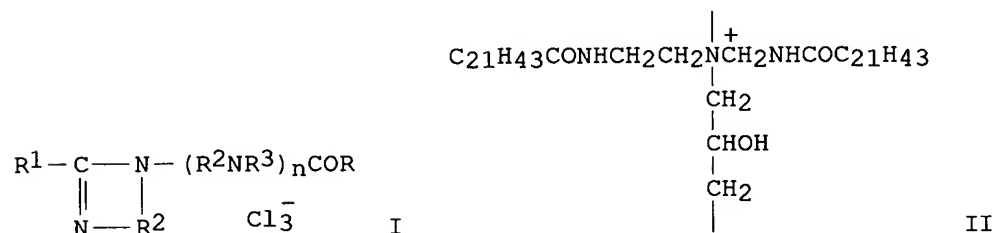
LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 03193980	A2	19910823	JP 1989-328872	19891218
PRIORITY APPLN. INFO.:			JP 1989-328872	19891218

GI



AB Leather-like sheets with good feel and tear strength are prepared by incorporating 0.1-3.0% cationic activating agent to nonwoven sheets (fiber fineness 0.001-3 denier), impregnating with an elastic polymer and wet coagulating, where the activating agent is derived from epichlorohydrin and polyamine derivs. I or R1CONR3(R2NR3)COR (R, R = C11-25 alkyl; R2 = C2-3 alkylene; R3 = H or crosslinking bond; n = 1-8). Needle punching a mixed web of PET and polyethylene, hot pressing at 120°, removing polyethylene component using C2Cl4, fibrillating, treating with a 0.7% aqueous solution of II, impregnating with 13% DMF solution of polyurethane elastomer, coagulating in a 50/50 aqueous DMF, and puffing gave a 1-mm suede leather substitute.

IT 137955-63-6

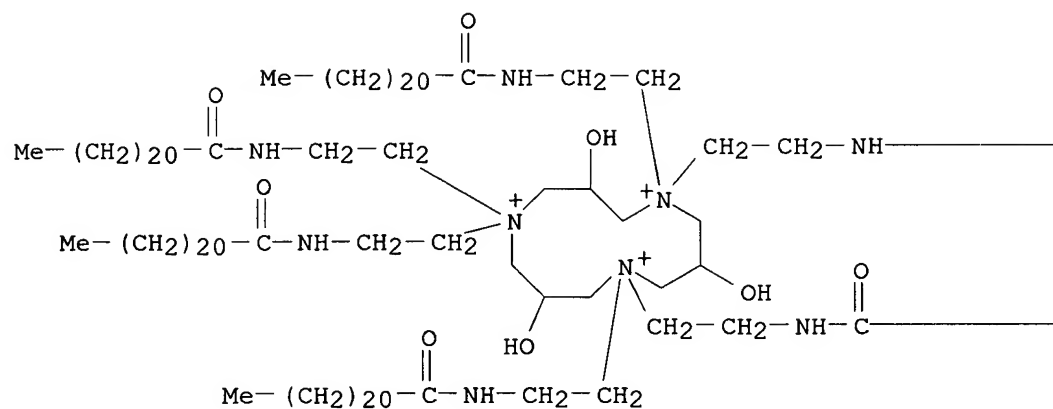
RL: USES (Uses)

(activating agents, in manufacture of leather substitutes with good feel and tear strength)

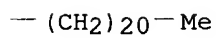
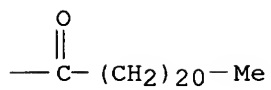
RN 137955-63-6 CAPLUS

CN 1,5,9-Triazoniacyclododecane, 3,7,11-trihydroxy-1,1,5,5,9,9-hexakis[2-[(1-oxodocosyl)amino]ethyl]-, trichloride (9CI) (CA INDEX NAME)

PAGE 1-A

● 3 Cl⁻

PAGE 1-B



130 ANSWER 64 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1991:548941 CAPLUS

DOCUMENT NUMBER: 115:148941

TITLE: Macrocyclic ligands designed to impose tetrahedral coordination: [1-(3-dimethylaminopropyl)-1,5,9-triazacyclododecane], L1, [1{2-(pyrrolidin-1-yl)ethyl}-1,5,9-triazacyclododecane], L2, and their zinc(II) complexes

AUTHOR(S): Alcock, Nathaniel W.; Benniston, Andrew C.; Moore, Peter; Pike, Graham A.; Rawle, Simon C.

CORPORATE SOURCE: Dep. Chem., University of Warwick, Coventry, CV4 7AL, UK

SOURCE: Journal of the Chemical Society, Chemical Communications (1991), (10), 706-8
CODEN: JCCCAT; ISSN: 0022-4936

DOCUMENT TYPE: Journal

LANGUAGE: English

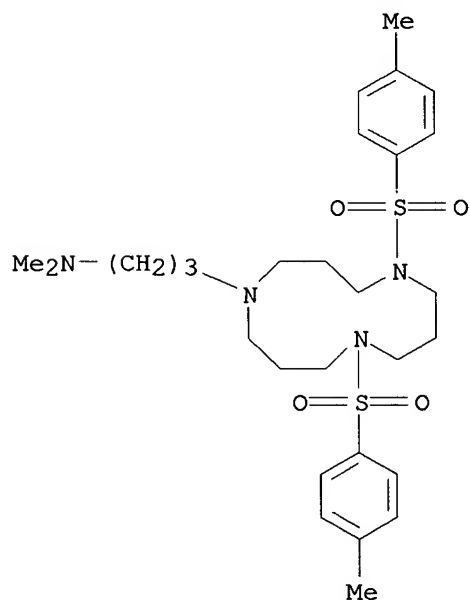
AB L (1-R-1,5,9-triaacyclododecane; R = Me₂NCH₂CH₂CH₂, QCH₂CH₂; Q = pyrrolidin-1-yl) were prepared L reacted with [Zn(DMSO)₄](ClO₄)₂ to yield ZnL(ClO₄)₂, which were characterized by x-ray crystallog. [Zn(L1)(ClO₄)₂ (I; L1 = L (R = Me₂NCH₂CH₂CH₂)) crystallizes as orthorhombic, space group Pcab, a 15.054(8), b 15.34(1), c 19.25(1) Å, Z = 8, R = 0.0750. [Zn(L2)(OCLO₃)]ClO₄ (II; L2 = L (R = QCH₂CH₂)) crystallizes as orthorhombic, space group Pn21a, a 13.875(13), b 9.811(6), c 16.186(9) Å, Z = 4, R = 0.0570. The Zn in I is approx. tetrahedrally coordinated by L1. The Zn in II has distorted trigonal bipyramid coordination by L2 and OCLO₃-.

IT 135787-24-5P 135787-25-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and detosylation of)

RN 135787-24-5 CAPLUS

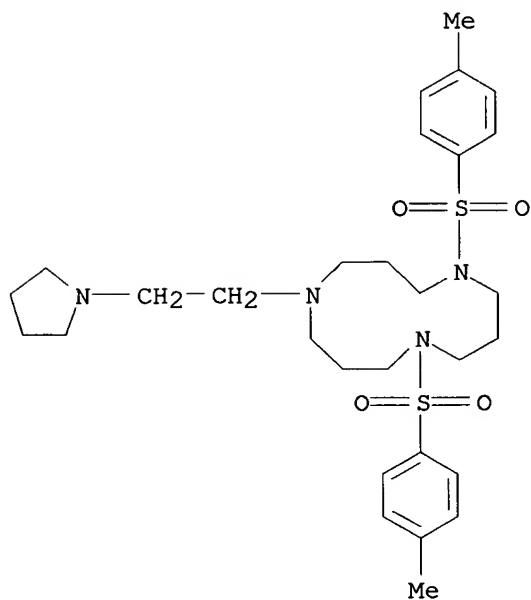
CN 1,5,9-Triazacyclododecane-1-propanamine, N,N-dimethyl-5,9-bis[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)



10/680,076

RN 135787-25-6 CAPLUS

CN 1,5,9-Triazacyclododecane, 1,5-bis[(4-methylphenyl)sulfonyl]-9-[2-(1-pyrrolidinyl)ethyl]- (9CI) (CA INDEX NAME)



~~D30~~ ANSWER 65 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1991:109632 CAPLUS

DOCUMENT NUMBER: 114:109632

TITLE: Preparation of terephthaloyl derivatives of cyclic triamines and their selectivities toward copper(II), nickel(II) and zinc(II) ions

AUTHOR(S): Fujiwara, Manabu; Matsuda, Jun; Wakita, Hisanobu

CORPORATE SOURCE: Fac. Sci., Fukuoka Univ., Fukuoka, 814-01, Japan

SOURCE: Polyhedron (1990), 9(20), 2491-5

CODEN: PLYHDE; ISSN: 0277-5387

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Three polymeric ligands containing 9-, 10- and 12-membered cyclic triamines were prepared by the reaction of cyclic triamine with terephthaloyl chloride. They are insol. in water and ordinary organic solvents, but under heterogeneous conditions they can adsorb some transition metal ions [Cu(II), Ni(II), and Zn(II)] very rapidly. The complexing abilities of the 9- and 10-membered polymeric ligands are stronger in the order Zn < Ni < Cu, but that of the 12-membered polymeric ligand is Ni < Zn < Cu.

IT 132434-02-7P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and selective capacity for transition metals of)

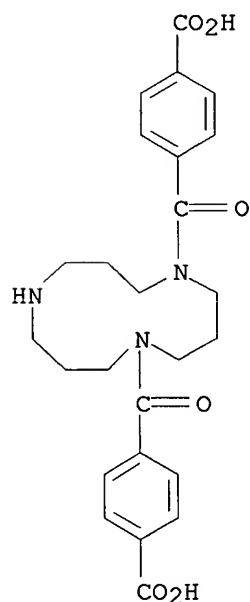
RN 132434-02-7 CAPLUS

CN Benzoic acid, 4,4'-(1,5,9-triazacyclododecane-1,5-diylldicarbonyl)bis-, homopolymer (9CI) (CA INDEX NAME)

CM 1

CRN 132434-01-6

CMF C25 H29 N3 O6



130 ANSWER 66 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1991:30923 CAPLUS

DOCUMENT NUMBER: 114:30923

TITLE: Synthesis and binding properties of amide-functionalized polyaza macrocycles

AUTHOR(S): Katakya, Ritu; Matthes, Karen E.; Nicholson, Patrick E.; Parker, David; Buschmann, Hans J.

CORPORATE SOURCE: Dep. Chem., Univ. Durham, Durham, DH1 3LE, UK

SOURCE: Journal of the Chemical Society, Perkin Transactions 2: Physical Organic Chemistry (1972-1999) (1990), (8), 1425-32

CODEN: JCPKBH; ISSN: 0300-9580

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 114:30923

AB A series of amide N-functionalized coronands was prepared based on parent [9]-N3, [12]-N3, [12]-N2O2, and [12]-N4 polyazamacrocycles. Complexation with alkali and alkaline earth cations, particularly Li⁺, Na⁺, and Ca²⁺, was monitored by using ¹³C NMR and IR spectroscopy, fast-atom-bombardment mass spectrometry, calorimetric, and potentiometric anal. in aqueous and alc. media. Particularly strong complexation in H₂O was observed for Ca²⁺ with 1,4,7,10-tetrakis(N,N-dimethylacetamido)-1,4,7,10-tetraazacyclododecane (log K_s = 6.82 [H₂O, 298 K]), and selective Ca²⁺ complexation was observed with 1,7-dioxa-4,10-bis(dimethylethanamido)-4,10-diazacyclododecane.

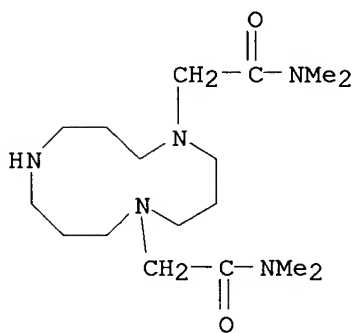
IT 127603-39-8

RL: PRP (Properties)

(acid dissociation consts. of)

RN 127603-39-8 CAPLUS

CN 1,5,9-Triazacyclododecane-1,5-diacetamide, N,N,N',N'-tetramethyl- (9CI)
(CA INDEX NAME)



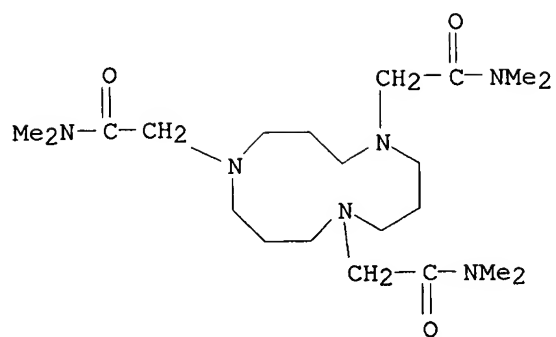
IT 127603-41-2D, lithium and sodium complexes

RL: PRP (Properties)

(selectivity in formation and stability consts. of)

RN 127603-41-2 CAPLUS

CN 1,5,9-Triazacyclododecane-1,5,9-triacetamide, N,N,N',N',N'',N''-hexamethyl- (9CI) (CA INDEX NAME)



10/680,076

~~130~~ ANSWER 67 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1991:7349 CAPLUS

DOCUMENT NUMBER: 114:7349

TITLE: Polycondensation catalyzed by palladium complex. III.
Syntheses of linear polyamines and cyclic oligoamines
via π -allyl palladium intermediates

AUTHOR(S): Suzuki, Masato; Lim, Jong Chan; Oguni, Masahiro;
Eberhardt, Anke; Saegusa, Takeo

CORPORATE SOURCE: Fac. Eng., Kyoto Univ., Kyoto, 606, Japan

SOURCE: Polymer Journal (Tokyo, Japan) (1990), 22(9), 815-25

CODEN: POLJB8; ISSN: 0032-3896

DOCUMENT TYPE: Journal

LANGUAGE: English

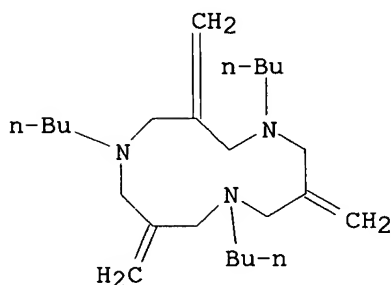
AB Polyamines were prepared by polymerization of bifunctional allylic compds. with
diamines or monoamines in the presence of Pd complexes. Tosylated amines
were also used to produce the corresponding tosylated derivs. of
polyamines. The monomer structure and the character of the catalyst
influenced the proportion between linear and cyclic products.

IT 130927-29-6P 130927-35-4P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 130927-29-6 CAPLUS

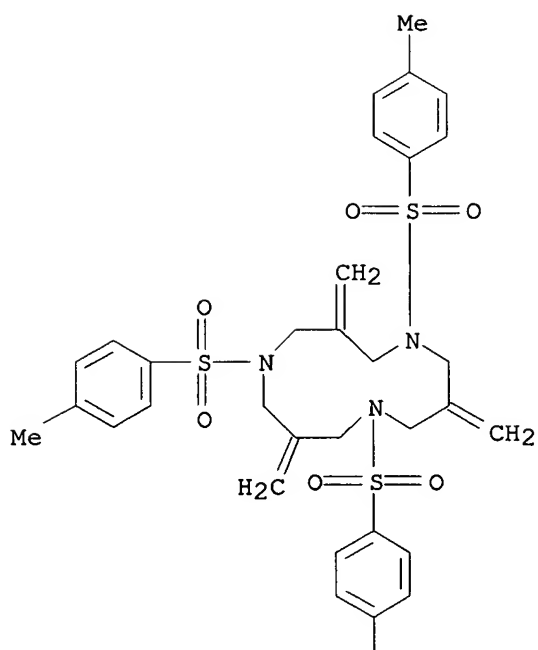
CN 1,5,9-Triazacyclododecane, 1,5,9-tributyl-3,7,11-tris(methylene)- (9CI)
(CA INDEX NAME)



RN 130927-35-4 CAPLUS

CN 1,5,9-Triazacyclododecane, 3,7,11-tris(methylene)-1,5,9-tris[(4-
methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 2-A



10/680,076

130 ANSWER 68 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1990:571994 CAPLUS

DOCUMENT NUMBER: 113:171994

TITLE: Macroheterocycles. 51. Synthesis of macrocyclic polyamines in a two-phase system

AUTHOR(S): Luk'yanenko, N. G.; Basok, S. S.; Filonova, L. K.; Kulikov, N. V.; Pastushok, V. N.

CORPORATE SOURCE: Fiz.-Khim. Inst., Odessa, 270080, USSR

SOURCE: Khimiya Geterotsiklicheskikh Soedinenii (1990), (3), 401-4

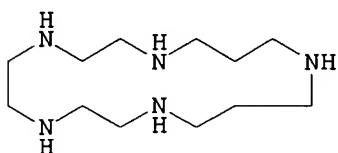
CODEN: KGSSAQ; ISSN: 0453-8234

DOCUMENT TYPE: Journal

LANGUAGE: Russian

OTHER SOURCE(S): CASREACT 113:171994

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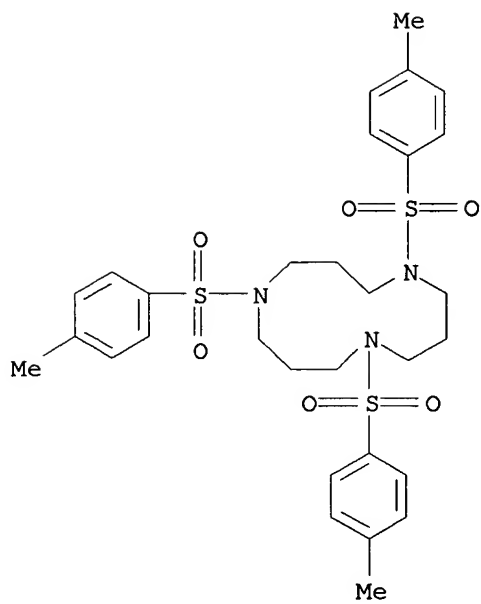
AB A new convenient synthesis of macrocyclic polyamines e.g., (I) based on condensation of bis(sulfonamides) with bis(tosylates) or dibromides in a two-phase toluene(xylene)-aqueous NaOH system gives the title compds. in 65-90% yield.

IT 35980-67-7P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and detosylation of)

RN 35980-67-7 CAPLUS

CN 1,5,9-Triazacyclododecane, 1,5,9-tris[(4-methylphenyl)sulfonyl]- (9CI)
(CA INDEX NAME)



~~L30~~ ANSWER 69 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1990:563133 CAPLUS

DOCUMENT NUMBER: 113:163133

TITLE: Liquid crystalline azamacrocyclic derivatives

AUTHOR(S): Lattermann, G.

CORPORATE SOURCE: Univ. Bayreuth, Bayreuth, D-8580, Germany

SOURCE: Molecular Crystals and Liquid Crystals (1990), 182B, 299-311

CODEN: MCLCA5; ISSN: 0026-8941

DOCUMENT TYPE: Journal

LANGUAGE: English

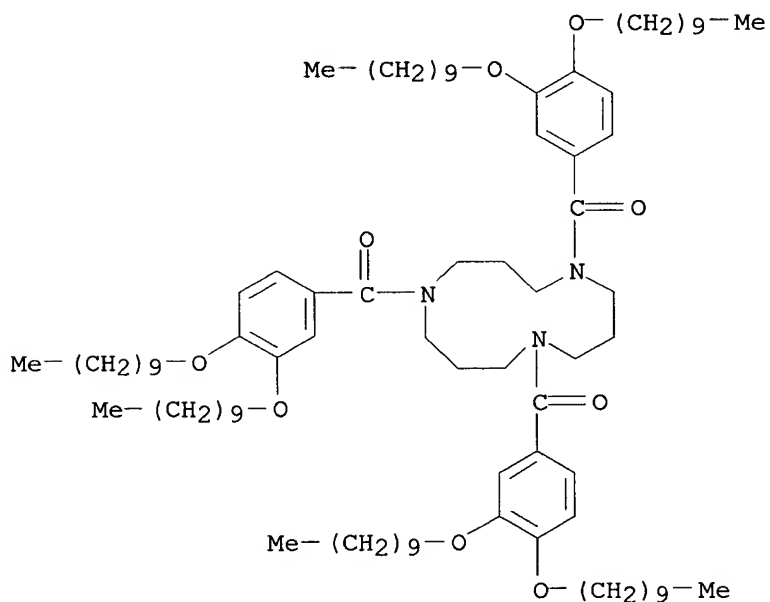
AB Three examples of new liquid crystalline compds. with azamacrocyclic cores are described. Apart from a substituted hexacyclene with 12 alkoxy sidechains, 2 triazacrown ether derivs. are presented. Their discotic mol. shape causes mesomorphic behavior, which is characterized by DSC-measurements and polarizing microscopy. Water absorption from air can slightly modify the transition temps. The triazamacrocyclic derivs. exhibit a strongly hindered recrystn.; their glass transition temps. are above room temperature

IT 129820-26-4P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(liquid crystal, preparation and transition temps. of)

RN 129820-26-4 CAPLUS

CN 1,5,9-Triazacyclododecane, 1,5,9-tris[3,4-bis(decyloxy)benzoyl]- (9CI)
(CA INDEX NAME)



10/680,076

130 ANSWER 70 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1990-423877 CAPLUS

DOCUMENT NUMBER: 113:23877

TITLE: Syntheses of C- and N-functionalized derivatives of 1,5,9-triazacyclododecane

AUTHOR(S): Helps, Ian M.; Parker, David; Jankowski, Karl J.; Chapman, James; Nicholson, Patrick E.

CORPORATE SOURCE: Dep. Chem., Univ. Durham, Durham, DH1 3LE, UK

SOURCE: Journal of the Chemical Society, Perkin Transactions

1: Organic and Bio-Organic Chemistry (1972-1999)

(1989), (11), 2079-82

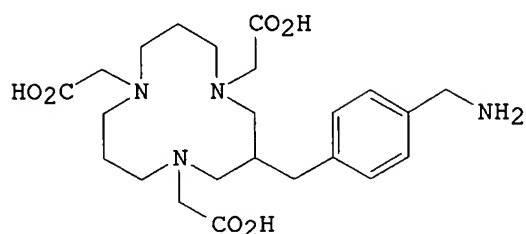
CODEN: JCPRB4; ISSN: 0300-922X

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 113:23877

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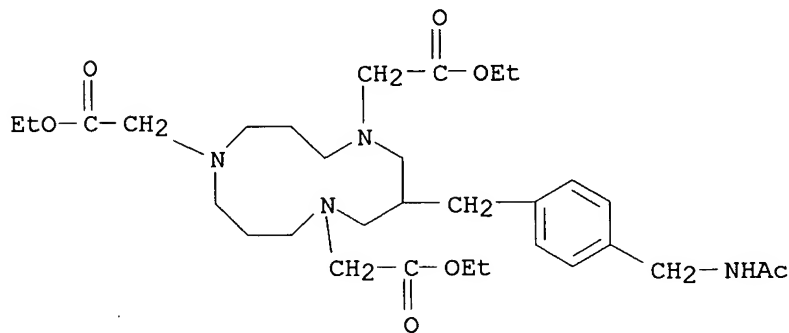
AB The synthesis of a series of di- and tri-N-substituted triazacyclododecane ligands has been effected through the intermediacy of monotosylamide derivs. A C-functionalized aminobenzyl [12]-N3 tris(carboxymethyl) derivative I has been prepared permitting subsequent linkage to a protein.

IT 124659-34-3P 127603-38-7P 127603-40-1P
127647-89-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and hydrolysis of)

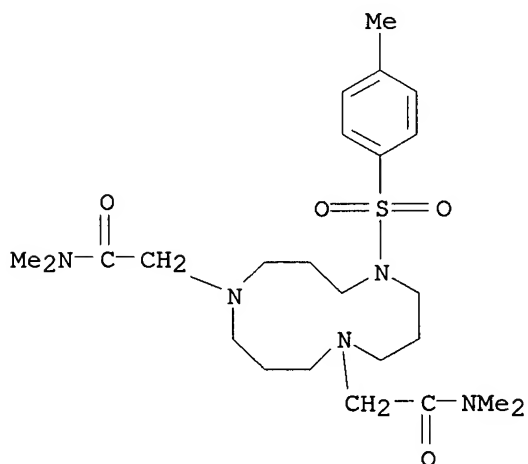
RN 124659-34-3 CAPLUS

CN 1,5,9-Triazacyclododecane-1,5,9-triacetic acid, 3-[[4-[(acetylamino)methyl]phenyl]methyl]-, triethyl ester (9CI) (CA INDEX NAME)



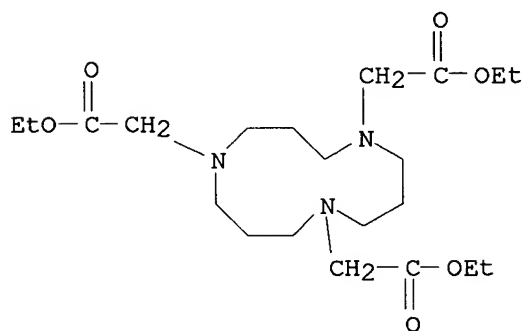
RN 127603-38-7 CAPLUS

CN 1,5,9-Triazacyclododecane-1,5-diacetamide, N,N,N',N'-tetramethyl-9-[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)



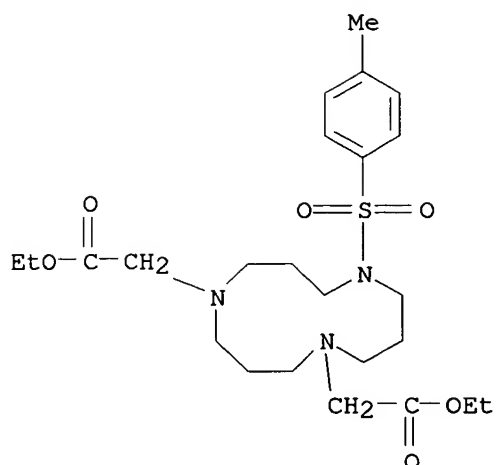
RN 127603-40-1 CAPLUS

CN 1,5,9-Triazacyclododecane-1,5,9-triacetic acid, triethyl ester (9CI) (CA INDEX NAME)



RN 127647-89-6 CAPLUS

CN 1,5,9-Triazacyclododecane-1,5-diacetic acid, 9-[(4-methylphenyl)sulfonyl]-, diethyl ester (9CI) (CA INDEX NAME)

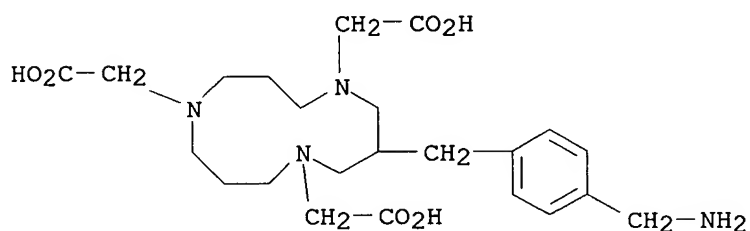


IT 124659-35-4P 127603-37-6P 127603-39-8P
127603-41-2P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

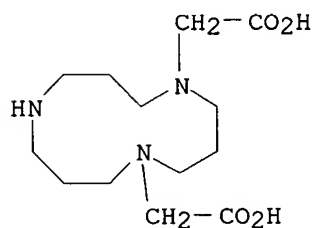
RN 124659-35-4 CAPLUS

CN 1,5,9-Triazacyclododecane-1,5,9-triacetic acid, 3-[[4-(aminomethyl)phenyl]methyl]- (9CI) (CA INDEX NAME)



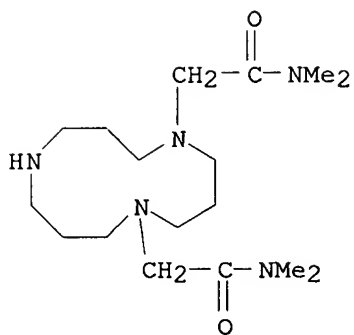
RN 127603-37-6 CAPLUS

CN 1,5,9-Triazacyclododecane-1,5-diacetic acid (9CI) (CA INDEX NAME)



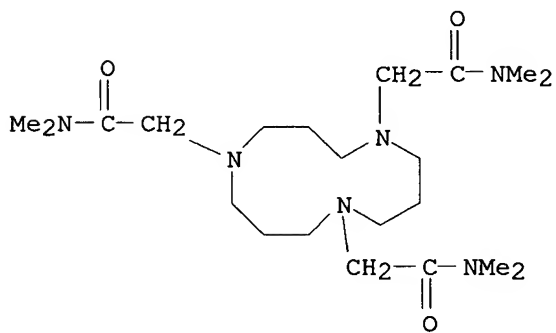
RN 127603-39-8 CAPLUS

CN 1,5,9-Triazacyclododecane-1,5-diacetamide, N,N,N',N'-tetramethyl- (9CI)
(CA INDEX NAME)



RN 127603-41-2 CAPLUS

CN 1,5,9-Triazacyclododecane-1,5,9-triacetamide, N,N,N',N',N'',N''-hexamethyl-
(9CI) (CA INDEX NAME)



130 ANSWER 71 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1990:118864 CAPLUS

DOCUMENT NUMBER: 112:118864

TITLE: Tri-aza macrocycles and metal complexes thereof, their preparation and use in diagnostic imaging and therapy

INVENTOR(S): Parker, David; Millican, Thomas Andrew

PATENT ASSIGNEE(S): Celltech Ltd., UK

SOURCE: PCT Int. Appl., 38 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

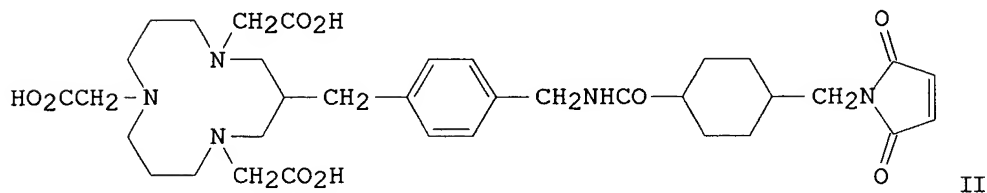
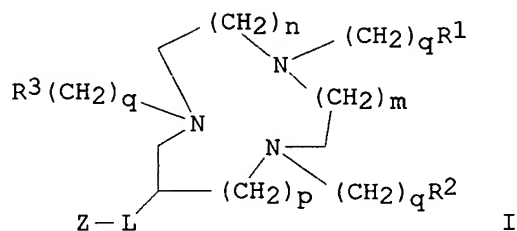
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 8901475	A1	19890223	WO 1988-GB672	19880812
W: AU, DK, JP, KR, US				
RW: AT, BE, CH, DE, FR, GB, IT, LU, NL, SE				
AU 8822527	A1	19890309	AU 1988-22527	19880812
AU 629178	B2	19921001		
EP 329737	A1	19890830	EP 1988-906973	19880812
EP 329737	B1	19950412		
R: AT, BE, CH, DE, FR, GB, IT, LI, LU, NL, SE				
JP 02501069	T2	19900412	JP 1988-506687	19880812
AT 121082	E	19950415	AT 1988-906973	19880812
CA 1340603	A1	19990622	CA 1988-574629	19880812
DK 8901728	A	19890411	DK 1989-1728	19890411
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PRIORITY APPLN. INFO.:			GB 1987-19041	A 19870812
			WO 1988-GB672	A 19880812
			US 1989-363683	B1 19890609
			US 1991-784601	A3 19911022

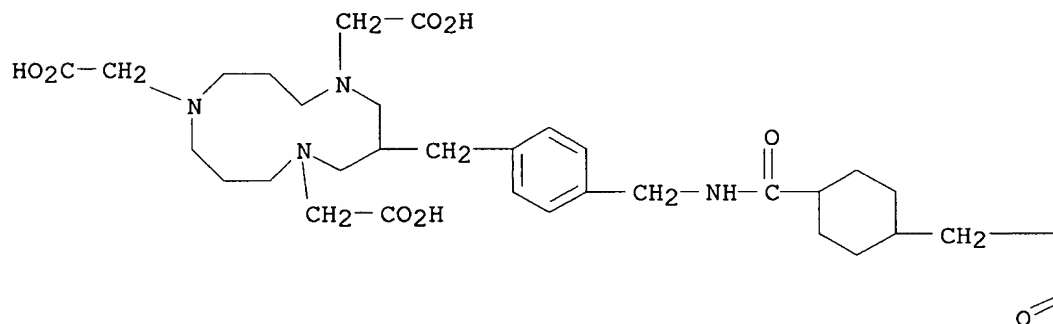
OTHER SOURCE(S): MARPAT 112:118864

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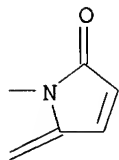


- AB Triazacycloalkane derivs. I (m, n = 0-3; p = 0-2; q = 0-6; R1-R3 = H, alkyl, alkoxyalkyl, CO₂H, SO₃H, PO₃H₂, aryl; L = bond, linker; Z = H, reactive functional group) and their metal complexes and salts are prepared for use in diagnostic imaging and treatment of abnormal cell disorders, e.g. tumors. I are particularly suitable for coupling to other mols. such as proteins for these applications. Thus, II was prepared in 8 steps from p-cyanobenzyl diethyl malonate and 1,7-diamino-4-azaheptane, converted to the ¹¹¹In complex, and conjugated with monoclonal antibody B72.3. When injected into mice, this conjugate showed high persistence in the tissues (≈65% of injected dose after 24 h), mainly in the blood (47.52%).
- IT 124659-23-0P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation and conjugation with monoclonal antibody for neoplasm inhibition and scintigraphy)
- RN 124659-23-0 CAPLUS
- CN 1,5,9-Triazacyclododecane-1,5,9-triacetic acid, 3-[[4-[[[4-[(2,5-dihydro-2,5-dioxo-1H-pyrrol-1-yl)methyl]cyclohexyl]carbonyl]amino]methyl]phenyl]methyl]- (9CI) (CA INDEX NAME)

PAGE 1-A



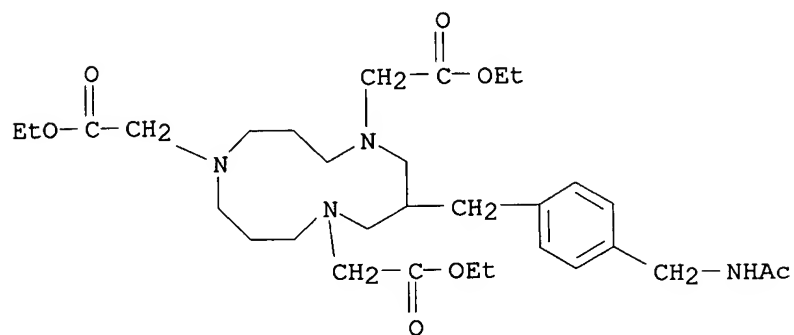
PAGE 1-B



- IT 124659-34-3P 124659-35-4P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of, in triazacyclononane derivative metal complex preparation as imaging agent and neoplasm inhibitor)
- RN 124659-34-3 CAPLUS
- CN 1,5,9-Triazacyclododecane-1,5,9-triacetic acid, 3-[[4-

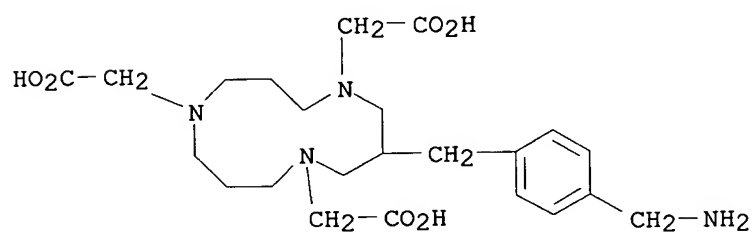
10/680,076

[(acetylamino)methyl]phenyl)methyl]-, triethyl ester (9CI) (CA INDEX NAME)



RN 124659-35-4 CAPLUS

CN 1,5,9-Triazacyclododecane-1,5,9-triacetic acid, 3-[[4-(aminomethyl)phenyl]methyl]- (9CI) (CA INDEX NAME)



L30 ANSWER 72 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1990:55813 CAPLUS

DOCUMENT NUMBER: 112:55813

TITLE: Towards tumor imaging with indium-111 labeled macrocycle-antibody conjugates

AUTHOR(S): Craig, Andrew S.; Helps, Ian M.; Jankowski, Karl J.; Parker, David; Beeley, Nigel R. A.; Boyce, Byron A.; Eaton, Michael A. W.; Millican, Andrew T.; Millar, Kenneth; et al.

CORPORATE SOURCE: Dep. Chem., Univ. Durham, Durham, DH1 3LE, UK

SOURCE: Journal of the Chemical Society, Chemical

Communications (1989), (12), 794-6

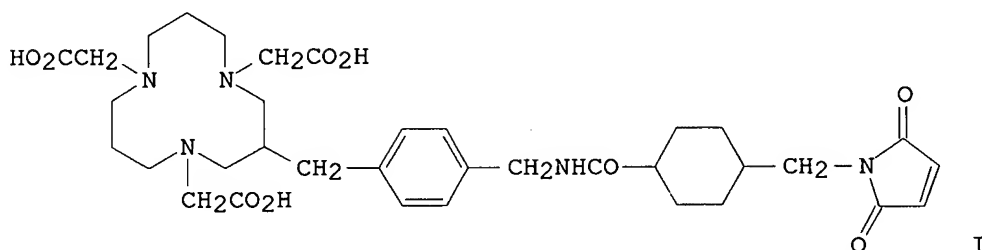
CODEN: JCCCAT; ISSN: 0022-4936

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 112:55813

GI



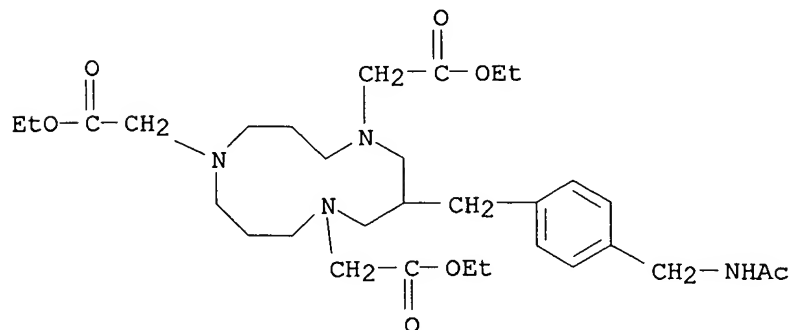
AB C-Functionalized triazacyclododecane and triazacyclononane triacid macrocycles, e.g. I, have been prepared and covalently attached to a monoclonal antibody and may be labeled with ¹¹¹In to form kinetically inert radiolabeled complexes.

IT 124659-34-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and acid hydrolysis of)

RN 124659-34-3 CAPLUS

CN 1,5,9-Triazacyclododecane-1,5,9-triacetic acid, 3-[[4-[(acetylamino)methyl]phenyl]methyl]-, triethyl ester (9CI) (CA INDEX NAME)



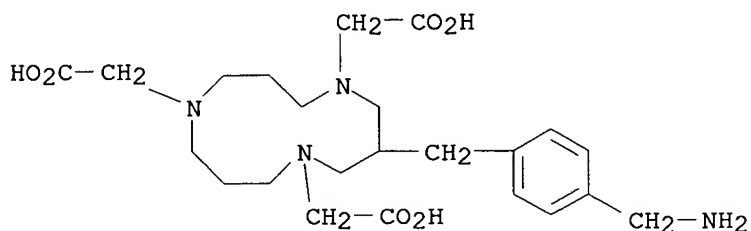
IT 124659-35-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and amidation by, of (carboxycyclohexylmethyl)maleimide)

RN 124659-35-4 CAPLUS

CN 1,5,9-Triazacyclododecane-1,5,9-triacetic acid, 3-[[4-(aminomethyl)phenyl]methyl]- (9CI) (CA INDEX NAME)

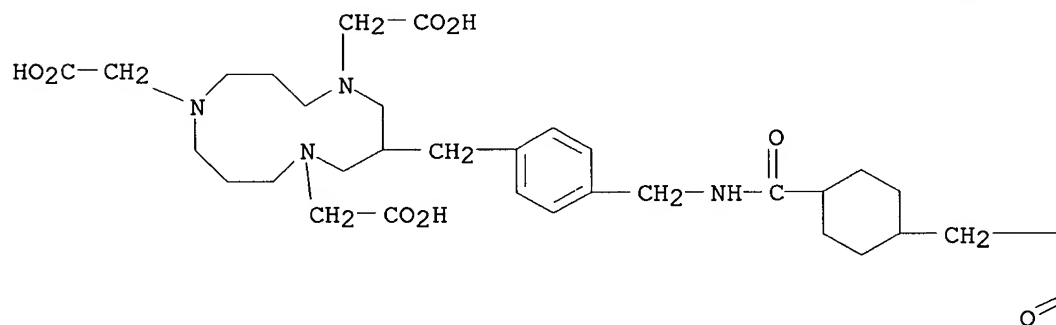


IT 124659-23-0P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and complexation of, with indium-111 trichloride)

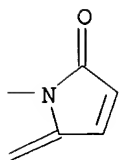
RN 124659-23-0 CAPLUS

CN 1,5,9-Triazacyclododecane-1,5,9-triacetic acid, 3-[[4-[[[4-[(2,5-dihydro-2,5-dioxo-1H-pyrrol-1-yl)methyl]cyclohexyl]carbonyl]amino]methyl]phenyl]methyl]- (9CI) (CA INDEX NAME)



PAGE 1-A

PAGE 1-B



10/680,076

190 ANSWER 73 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1990:26399 CAPLUS

DOCUMENT NUMBER: 112:26399

TITLE: Potentiometry and NMR studies of 1,5,9-triazacyclododecane-N,N',N''-triacetic acid and its metal ion complexes

AUTHOR(S): Cortes, S.; Brucher, E.; Gerald, C. F. G. C.; Sherry, A. D.

CORPORATE SOURCE: Univ. Texas, Dallas, Richardson, TX, 75083-0688, USA

SOURCE: Inorganic Chemistry (1990), 29(1), 5-9

CODEN: INOCAJ; ISSN: 0020-1669

DOCUMENT TYPE: Journal

LANGUAGE: English

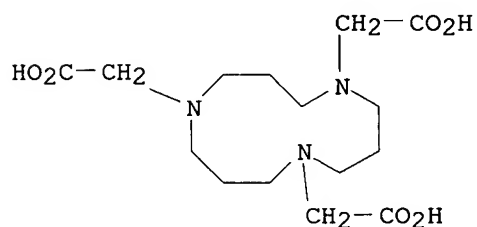
AB A new chelating macrocycle, 1,5,9-triazacyclododecane-N,N',N''-triacetic acid (DOTRA), has been synthesized, and its complexes with Zn²⁺, Cd²⁺, Ca²⁺, Mg²⁺, and Mn²⁺ have been examined by potentiometry and NMR spectroscopy. The first protonation constant of the free ligand (log K₁ = 12.8) was determined spectrophotometrically, while the remaining were evaluated from potentiometric data (log K₂ = 7.55, log K₃ = 3.65, log K₄ = 2.1). DOTRA forms complexes with Mn²⁺, Mg²⁺, and Ca²⁺ rather slowly but reacts much more rapidly with Zn²⁺ and Cd²⁺. As reported previously for the nine-membered-ring triaza analog NOTA, DOTRA also forms a more stable complex with Mg²⁺ than with Ca²⁺ (log K_{st} = 7.1 vs. 6.0). High-resolution NMR spectra of the Zn²⁺, Cd²⁺, and Mg²⁺ complexes (log K_{st} = 19.0, 15.7, and 7.1, resp.) indicate the three six-membered chelate rings are sym. and quite rigid in aqueous solution, as evidenced by nonequivalence of all six chelate ring protons.

IT 123726-20-5P 123726-21-6P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 123726-20-5 CAPLUS

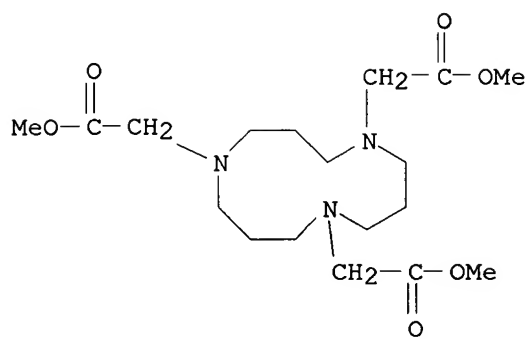
CN 1,5,9-Triazacyclododecane-1,5,9-triacetic acid, trihydrochloride (9CI)
(CA INDEX NAME)



⊕3 HCl

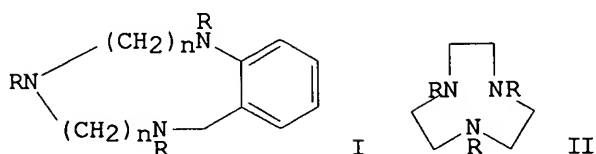
RN 123726-21-6 CAPLUS

CN 1,5,9-Triazacyclododecane-1,5,9-triacetic acid, trimethyl ester (9CI) (CA INDEX NAME)



10/680,076

130 ANSWER 74 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1989:407379 CAPLUS
DOCUMENT NUMBER: 111:7379
TITLE: A simplified synthetic route to polyaza macrocycles
AUTHOR(S): Chavez, F.; Sherry, A. D.
CORPORATE SOURCE: Dep. Chem., Univ. Texas, Dallas, Richardson, TX,
75083-0688, USA
SOURCE: Journal of Organic Chemistry (1989), 54(12), 2990-2
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 111:7379
GI



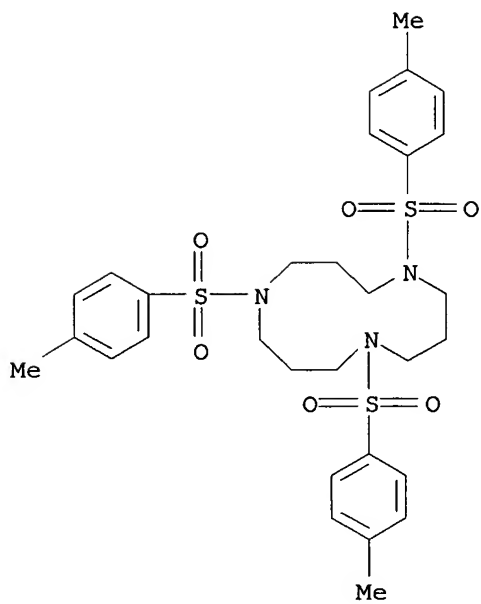
AB A simple, low-cost procedure for the preparation of small to medium-sized polyazamacrocycles, e.g. I ($n = 2, 3$; $R = \text{tosyl}$) and II ($R = \text{tosyl}$) is reported. It involves base deprotonation of a linear polyazatosylamide by finely ground K_2CO_3 in dry DMF followed by slow addition of a dibromoalkane at or near room temperature. The reaction may be run at final concns. approaching 0.1M on gram or multigram scales and with yields, after isolation and recrystn., approaching 90%.

IT 35980-67-7P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 35980-67-7 CAPLUS

CN 1,5,9-Triazacyclododecane, 1,5,9-tris[(4-methylphenyl)sulfonyl]- (9CI)
(CA INDEX NAME)



180 ANSWER 75 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1989:407370 CAPLUS

DOCUMENT NUMBER: 111:7370

TITLE: Macroheterocycles. Part 44. Facile synthesis of azacrown ethers and cryptands in a two-phase system
 AUTHOR(S): Lukyanenko, N. G.; Basok, S. S.; Filonova, L. K.
 CORPORATE SOURCE: A. V. Bogatskii Phys.-Chem. Inst., Odessa, 270080, USSR

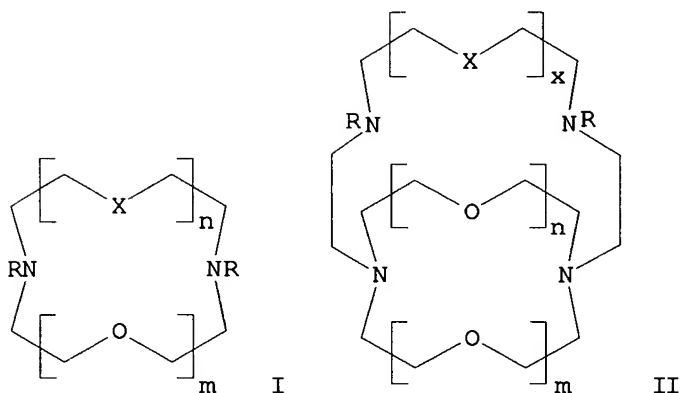
SOURCE: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (1988), (12), 3141-7
 CODEN: JCPRB4; ISSN: 0300-922X

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 111:7370

GI



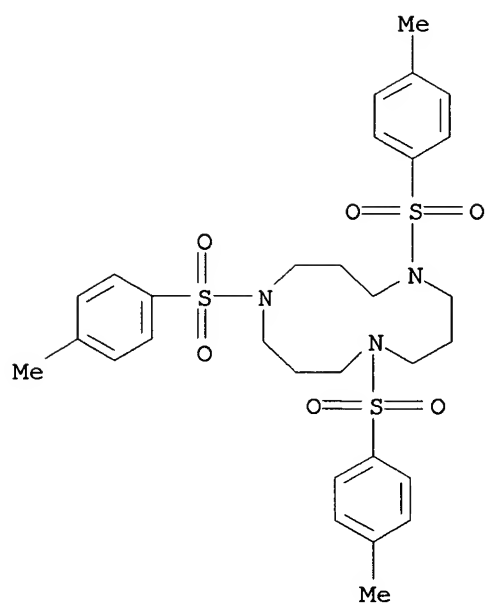
AB A facile procedure is proposed for the preparation of azacrown ethers, e.g., I (X = O, NR; R = tosyl, n, m = 1,2,3) and cryptands, e.g., II (X = O, NR; R = tosyl, n, m, x = 1,2) by condensation of dibromides or ethylene glycol bis(toluene-p-sulfonate) with acyclic bis(sulfonamide)s or with bis[2-(p-tolylsulfonylamino)ethyl]diazacrown ethers, resp. The reaction was carried out in a two-phase system of aqueous alkali-toluene (benzene) in the presence of quaternary ammonium salts as phase transfer catalysts. The catalytic activity decreased in the sequence: Bu4Nl ≈ Bu4NBr > Bu4NCl > Bu4NHSO4 > Et3CH2C6H5NCl. Maximum yields of twelve-membered azacrown ethers are obtained when lithium hydroxide is used, while crown ethers of larger size are observed in the presence of sodium or potassium hydroxides; this may be due to a template effect.

IT 35980-67-7P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation and detosylation of)

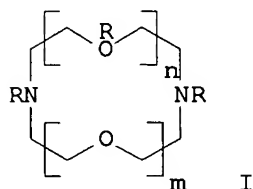
RN 35980-67-7 CAPLUS

CN 1,5,9-Triazacyclododecane, 1,5,9-tris[(4-methylphenyl)sulfonyl]- (9CI)
 (CA INDEX NAME)



10/680,076

130 ANSWER 76 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1989:231598 CAPLUS
DOCUMENT NUMBER: 110:231598
TITLE: Macroheterocycles. XXXVI. Convenient synthesis of
di- and polyaza crown ethers
AUTHOR(S): Luk'yanenko, N. G.; Bosok, S. S.; Filonova, L. K.
CORPORATE SOURCE: Fiz.-Khim. Inst. im. Bogatskogo, Odessa, USSR
SOURCE: Zhurnal Organicheskoi Khimii (1988), 24(8), 1731-42
CODEN: ZORKAE; ISSN: 0514-7492
DOCUMENT TYPE: Journal
LANGUAGE: Russian
OTHER SOURCE(S): CASREACT 110:231598
GI



AB Di- and polyaza crown ethers, e.g. I (R = tosyl, H, n, m = 0-8) were prepared by condensation of bissulfonamides with dibromides and ditosylates in a 2-phase system containing aqueous base and either toluene or C₆H₆. The optimum concentration range for the substrate and alkylating agent are 0.017-0.1 mol/L. The catalytic activity of the quaternary ammonium salts decrease in the series: Bu₄NI ≥ Bu₄NCl > Bu₄NHSO₄ > Et₃PhCH₂NCl ≥ Et₄NI > Et₄NBr. The maximum yield of 12 crown ethers were obtained with LiOH solns.; with the remainder NaOH and KOH are favored.

IT 35980-67-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and hydrolysis of)

RN 35980-67-7 CAPLUS

CN 1,5,9-Triazacyclododecane, 1,5,9-tris[(4-methylphenyl)sulfonyl]- (9CI)
(CA INDEX NAME)

10/680,076

LIBRARY ANSWER 77 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1988:94528 CAPLUS

DOCUMENT NUMBER: 108:94528

TITLE: Synthesis and copper(I) complexes of a series of 9- to 13-membered N3 macrocycles

AUTHOR(S): Briellmann, Markus; Kaderli, Susan; Meyer, Charles J.; Zuberbuhler, Andreas D.

CORPORATE SOURCE: Inst. Anorg. Chem., Univ. Basel, Basel, CH-4056, Switz.

SOURCE: Helvetica Chimica Acta (1987), 70(3), 680-9
CODEN: HCACAV; ISSN: 0018-019X

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 108:94528

GI For diagram(s), see printed CA Issue.

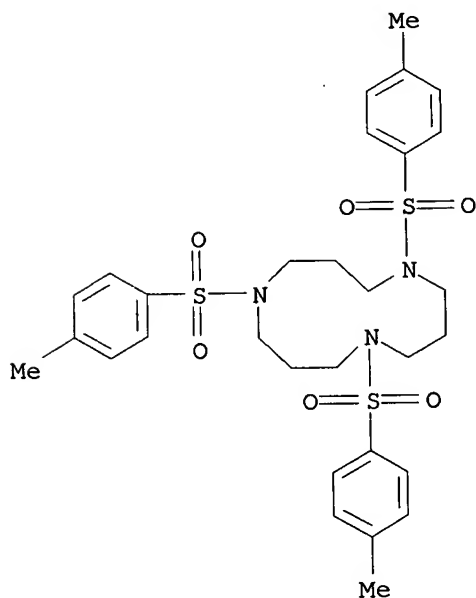
AB Eight cyclic triamines with ring sizes between 9 and 13 (I, n = 2, m = 2-6; n = 3, m = 2-4) were prepared by cyclocondensation of the appropriate triamine tritosylate with the appropriate ditosylate and subsequent detosylation of the macrocyclic triamine tritosylates.

IT 35980-67-7P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and detosylation of, with sulfuric acid)

RN 35980-67-7 CAPLUS

CN 1,5,9-Triazacyclododecane, 1,5,9-tris[(4-methylphenyl)sulfonyl]- (9CI)
(CA INDEX NAME)



10/680,076

L30 ANSWER 78 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1988:75328 CAPLUS

DOCUMENT NUMBER: 108:75328

TITLE: Synthesis of 2,3,5,6-tetrahydro-1H,4H,11cH-3a,6a,11b-triazabenz[de]anthracene (I) and x-ray crystal structure determinations of I, hexahydro-1H,4H,7H,9bH-3a,6a,9a-triazaphenalene, N,N',N''-tritosylbenzo[b]-[1,5,9]-triazacyclododecane, and of N,N',N''-tritosyl-1,5,9-triazacyclododecane

AUTHOR(S): Beddoes, Roy L.; Edwards, W. D.; Joule, J. A.; Mills, O. S.; Street, J. D.

CORPORATE SOURCE: Chem. Dep., Manchester Univ., Manchester, M13 9PL, UK

SOURCE: Tetrahedron (1987), 43(8), 1903-20

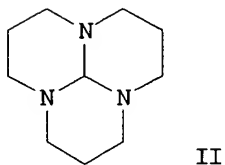
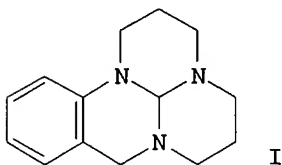
CODEN: TETRAB; ISSN: 0040-4020

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 108:75328

GI



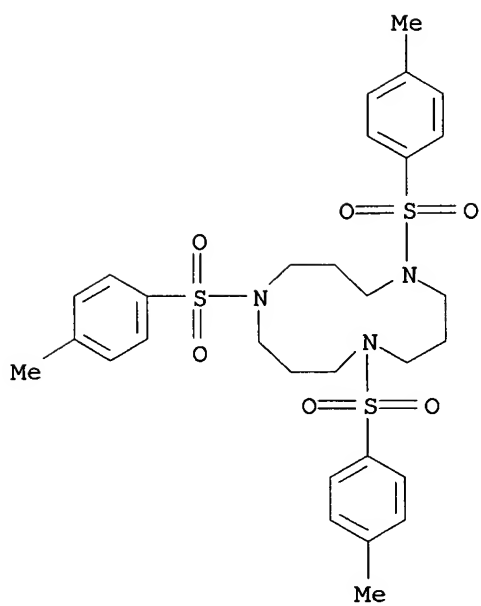
AB Triazabenz[de]anthracene I was prepared from anthranilonitrile. X-ray crystal structure detns. on triazaphenalene II and its benzo analog I show them to adopt differing conformations; the reasons for this are discussed.

IT 35980-67-7

RL: PRP (Properties)
(crystal structure of)

RN 35980-67-7 CAPLUS

CN 1,5,9-Triazacyclododecane, 1,5,9-tris[(4-methylphenyl)sulfonyl]- (9CI)
(CA INDEX NAME)



10/680,076

L30 ANSWER 79 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1988:56096 CAPLUS

DOCUMENT NUMBER: 108:56096

TITLE: Selective N-protection of medium-ring triamines

AUTHOR(S): Weisman, Gary R.; Vachon, David J.; Johnson, Van B.; Gronbeck, Dana A.

CORPORATE SOURCE: Dep. Chem., Univ. New Hampshire, Durham, NH, 03824, USA

SOURCE: Journal of the Chemical Society, Chemical Communications (1987), (12), 886-7

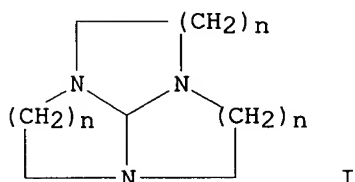
CODEN: JCCCAT; ISSN: 0022-4936

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 108:56096

GI



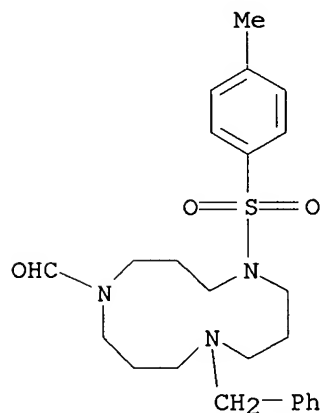
AB Efficient methods for selective N-protection of 1,4,7-triazacyclononane and 1,5,9-triazacyclododecane and for the synthesis of related bis(coronands) based upon the synthetic intermediacy of tricyclic ortho amides I (n = 1, 2) were developed.

IT 112498-56-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and hydrolysis of, by sodium hydroxide)

RN 112498-56-3 CAPLUS

CN 1,5,9-Triazacyclododecane-1-carboxaldehyde, 5-[(4-methylphenyl)sulfonyl]-9-(phenylmethyl)- (9CI) (CA INDEX NAME)

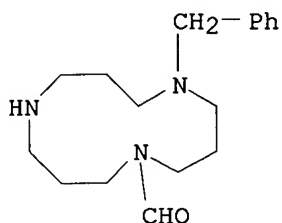


IT 112498-55-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(preparation and N-tosylation of)

RN 112498-55-2 CAPLUS

CN 1,5,9-Triazacyclododecane-1-carboxaldehyde, 5-(phenylmethyl)- (9CI) (CA
INDEX NAME)

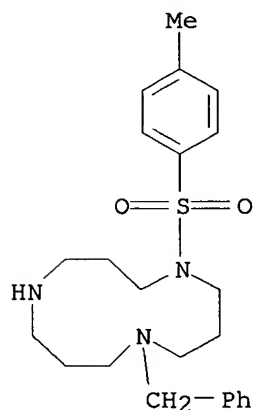


IT 112498-57-4P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 112498-57-4 CAPLUS

CN 1,5,9-Triazacyclododecane, 1-[(4-methylphenyl)sulfonyl]-5-(phenylmethyl)-
(9CI) (CA INDEX NAME)



L30 ANSWER 80 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1986:471514 CAPLUS

DOCUMENT NUMBER: 105:71514

TITLE: Synthesis and structure of metal complexes of triaza
macrocycles with three pendant pyridylmethyl armsAUTHOR(S): Christiansen, Lise; Hendrickson, David N.; Toftlund,
Hans; Wilson, Scott R.; Xie, Chuan Liang

CORPORATE SOURCE: Dep. Chem., Univ. Odense, Odense, DK-5230, Den.

SOURCE: Inorganic Chemistry (1986), 25(16), 2813-18

CODEN: INOCAJ; ISSN: 0020-1669

DOCUMENT TYPE: Journal

LANGUAGE: English

AB [ML](ClO₄)₂ and [CoL](ClO₄)₃ (L = 2,5,8-tris(2-pyridylmethyl)-2,5,8-triazanonane (L1); 1,4,7-tris(2-pyridylmethyl)-1,4,7-triazacyclononane (L2), 1,5,9-tris(2-pyridylmethyl)-1,5,9-triazacyclododecane (L3)) and the ligands were prepared. The x-ray structure of [FeL₂](ClO₄)₂ was determined by using Patterson methods, in conjunction with data measured on a 4-circle diffractometer, to give discrepancy factors of RF = 0.041 and RwF = 0.052 for 1841 observed ($I > 2.58\sigma(I)$) reflections. The compound crystallizes in the trigonal space group P3 with Z = 3, a 16.978(3) and c 7.909(3) Å. There are 3 crystallog. independent FeL₂ cations; each cation has a C3 axis perpendicular to the plane of the 3 pyridine N atoms as well as the plane of the 3 aliphatic N atoms of a L2 ligand. All 3 cations have similar dimensions; the bond distances are appropriate for a low-spin Fe(II) complex, a description that is in agreement with the variable-temperature

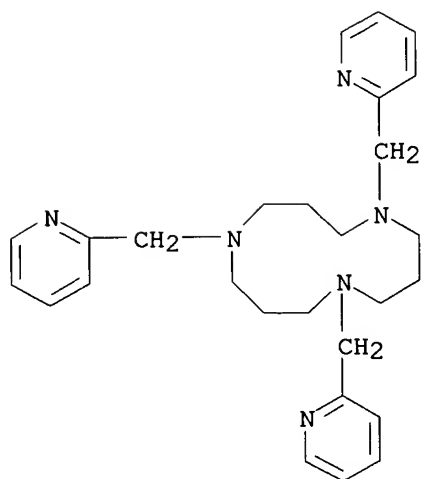
Moessbauer and magnetic susceptibility data that were obtained. The ClO₄- and SbF₆- salts of [FeL₁]²⁺ and [FeL₃]²⁺ are high-spin Fe(II) compds. Electronic absorption spectral data are presented for the [ML](ClO₄)₂ and [CoL](ClO₄)₃ in solution to show that the [FeL₂]²⁺ complex is close to the spin-crossover point. The interrelations between the kinetics of reactions such as racemization and the possibility of converting from low spin to high spin, i.e. the existence of the spin-crossover phenomenon, are examined for the L2 complex. ¹³C NMR results are presented to show that [FeL₂]²⁺ undergoes a relatively rapid racemization with a rate constant in excess of 150 s⁻¹ at 90°. The P3 is a polar space group, so the Fe(II) cations in [FeL₂](ClO₄)₂ are 1 of an enantiomeric pair; i.e., the cations are optically active and resolved. The kinetics of racemization that develop after a crushed large single crystal is dissolved, monitored with a CD spectrometer, give a rate constant of $k = 2.7 \times 10^{-3} \text{ s}^{-1}$ at 5°. The racemization takes place via an intramol. twist mechanism and such a mechanism is strongly favored by having a situation where the triplet excited state is close in energy to the singlet ground state of an Fe(II) complex.

IT 102851-51-4P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 102851-51-4 CAPLUS

CN 1,5,9-Triazacyclododecane, 1,5,9-tris(2-pyridinylmethyl)- (9CI) (CA INDEX
NAME)



ANSWER 81 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1986:207243 CAPLUS

DOCUMENT NUMBER: 104:207243

TITLE: I. Syntheses of selectively functionalized 9[ane]N3 and 12[ane]N3 cyclic triamines. II. Syntheses, complexation, and conformational studies of some azapodandocoronands

AUTHOR(S): Vachon, David John

CORPORATE SOURCE: Univ. New Hampshire, Durham, NH, USA

SOURCE: (1984) 321 pp. Avail.: Univ. Microfilms Int., Order No. DA8510484

From: Diss. Abstr. Int. B 1985, 46(3), 847

DOCUMENT TYPE: Dissertation

LANGUAGE: English

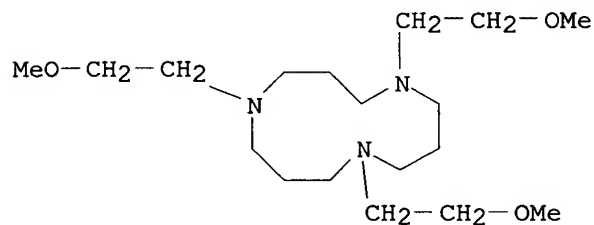
AB Unavailable

IT 102202-73-3P

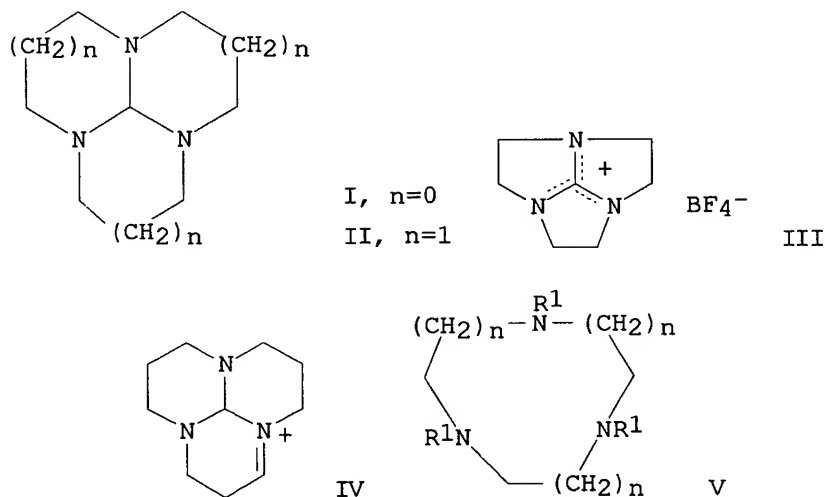
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation, complexation, and conformation of)

RN 102202-73-3 CAPLUS

CN 1,5,9-Triazacyclododecane, 1,5,9-tris(2-methoxyethyl)- (9CI) (CA INDEX NAME)



180 ANSWER 82 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN
 ACCESSION NUMBER: 1980:586289 CAPLUS
 DOCUMENT NUMBER: 93:186289
 TITLE: Transfer of hydrogen from orthoamides. Synthesis
 structure, and reactions of hexahydro-6bH-2a,4a,6a-
 triazacyclopenta[cd]pentalene and perhydro-3a,6a,9a-
 triazaphenalene
 AUTHOR(S): Erhardt, Jeanette M.; Grover, Edward R.; Wuest, James
 D.
 CORPORATE SOURCE: Dep. Chem., Harvard Univ., Cambridge, MA, 02138, USA
 SOURCE: Journal of the American Chemical Society (1980),
 102(20), 6365-9
 CODEN: JACSAT; ISSN: 0002-7863
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 93:186289
 GI

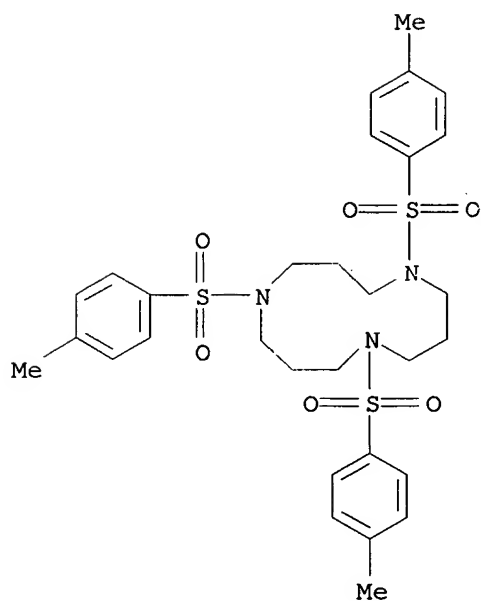


AB Hexahydro-6bH-2a,4a,6a-triazacyclopenta[c,d]pentalene (I) adopts a conformation in which the central C-H bond is syn-periplanar to three lone pairs; perhydro-3a,6a,9a-triazaphenalene (II) adopts a conformation in which the central C-H bond is anti-periplanar to three lone pairs. Orthoamide I readily reduces $\text{Ph}_3\text{C}^+ \text{BF}_4^-$ to Ph_3CH , and the product of oxidation is the guanidinium tetrafluoroborate III. Orthoamide II also reduces $\text{Ph}_3\text{C}^+ \text{BF}_4^-$ to Ph_3CH , but the central C-H bond is not broken: instead, steric or stereoelectronic factors appear to favor the formation of iminium ion IV. Both orthoamides efficiently reduce Me phenylglyoxylate in the presence of $\text{Mg}(\text{ClO}_4)_2$. I was prepared in 3 steps from triazonine V ($\text{R}^1 = \text{tosyl}$, $n = 1$) and II in 7 steps from $\text{HN}(\text{CH}_2\text{CH}_2\text{CO}_2\text{Et})_2$ via V ($\text{R}^1 = \text{tosyl}$, $n = 2$).

IT 35980-67-7P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation and reaction of, with hydrogen bromide)
 RN 35980-67-7 CAPLUS
 CN 1,5,9-Triazacyclododecane, 1,5,9-tris[(4-methylphenyl)sulfonyl]- (9CI)

10/680,076

(CA INDEX NAME)



10/680,076

L30 ANSWER 83 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1972:140751 CAPLUS

DOCUMENT NUMBER: 76:140751

TITLE: Syntheses of some medium-sized cyclic triamines and their cobalt(III) complexes

AUTHOR(S): Koyama, Hiroyuki; Yoshino, Tamotsu

CORPORATE SOURCE: Fac. Sci., Kyushu Univ., Fukuoka, Japan

SOURCE: Bulletin of the Chemical Society of Japan (1972), 45(2), 481-4

CODEN: BCSJA8; ISSN: 0009-2673

DOCUMENT TYPE: Journal

LANGUAGE: English

GI For diagram(s), see printed CA Issue.

AB Cyclic triamines (9-12-membered ring) form 3 mutually-adjacent 5-or 6-membered chelate rings on complexation, such as 1,4,7-triazacyclononane (I), 1,4,7-triazacyclodecane (II), 1,4,8-triazacycloundecane (III), and 1,5,9-triazacyclododecane (IV), which were isolated as their trihydrobromides. The complexation of I and II with a Co(III) salt gave metal complexes of a sandwich-type structure, such as $[\text{CoI}_2]\text{Br}_3$ and $[\text{CoII}_2]\text{Br}_3 \cdot \text{H}_2\text{O}$. In the case of III, a complex $[\text{CoIIIBrCl}_2]$ was isolated. Formation of a Co(III) complex with IV in solution was inferred spectroscopically but no expected complex was isolated. The ligand-field strength increased in the following order: $[\text{Co}(\text{NH}_3)_6]^{3+} < [\text{CoII}_2]^{3+} < [\text{Coen}_3]^{3+} < [\text{CoII}_2]^{3+}$.

IT 35980-67-7P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 35980-67-7 CAPLUS

CN 1,5,9-Triazacyclododecane, 1,5,9-tris[(4-methylphenyl)sulfonyl]- (9CI)
(CA INDEX NAME)

